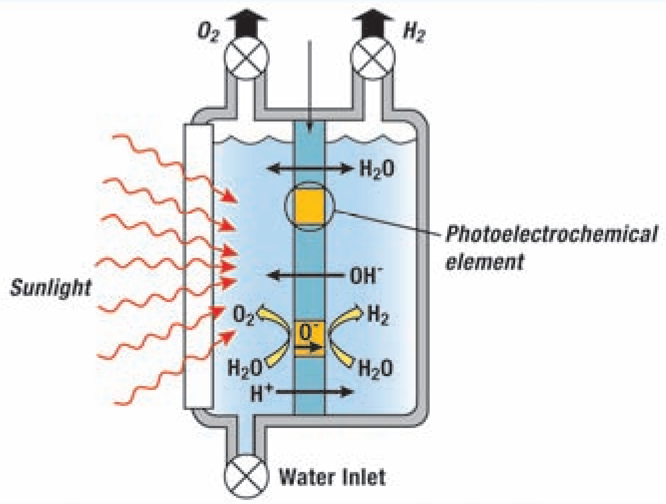
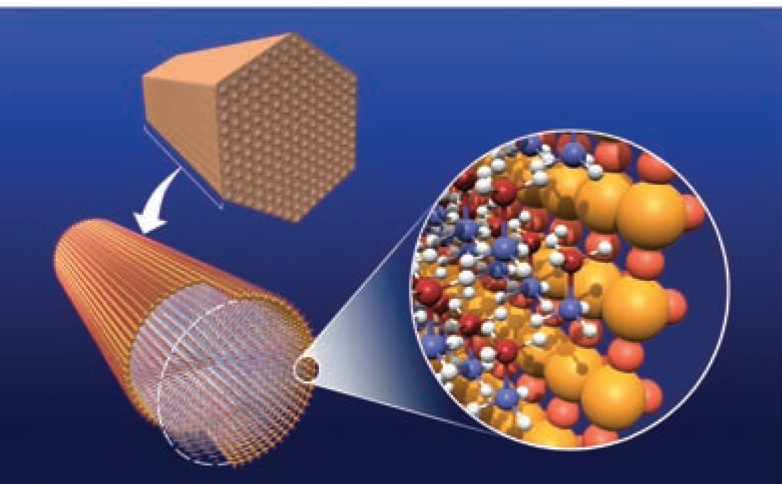
U.S. Department of Energy

DOE Hydrogen Program



May 15–18, 2007
Arlington, Virginia

2007 Annual Merit Review and Peer Evaluation Report



DOE/GO-102007-2476
September 2007

DOE Hydrogen Program

2007 Annual Merit Review and Peer Evaluation Report

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PROLOGUE

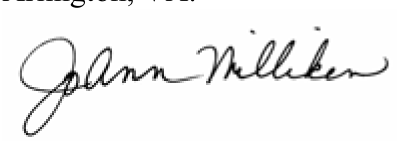
Dear Colleague:

This document summarizes the comments provided by the peer reviewers at the U.S. Department of Energy (DOE) Hydrogen Program's FY 2007 Annual Merit Review and Peer Evaluation meeting, held on May 14-18, 2007 in Washington, D.C. This review process provides evaluations of the Program's projects in applied research, technology development and demonstration, and analysis in response to direction from the Under Secretary of Energy. All four Offices that support the President's Hydrogen Fuel Initiative — Energy Efficiency and Renewable Energy (EERE), Fossil Energy (FE), Nuclear Energy (NE), and Science (SC) — participate in the meeting to provide the hydrogen community a view of the breadth and depth of DOE's efforts under the Initiative. In addition to the overview presentations given by all four Offices during the opening plenary session, projects from EERE, FE, and NE were presented and peer reviewed, and the fuel cell related projects from SC were provided as oral or poster presentations, but not evaluated by the reviewers.

The recommendations of the reviewers have been taken into consideration by DOE Technology Development Managers in the generation of future work plans. The table below lists the projects presented at the review, evaluation scores, and the major actions to be taken during the upcoming fiscal year (October 1, 2007 to September 30, 2008). The projects have been grouped according to Program Element (production, delivery, storage, fuel cells, etc.), and the weighted scores are based on a 4-point scale involving five criteria. To furnish all principal investigators (PIs) with direct feedback, all evaluations and comments are provided to each presenter; however, the authors of the individual comments remain anonymous. The PI of each project is instructed to fully consider these summary evaluation comments, as appropriate, in their FY 2008 plans.

I would like to express my sincere appreciation to the reviewers. It is they who make this report possible, and upon whose comments we rely to help make project decisions for the new fiscal year. Thank you for participating in the FY 2007 Annual Merit Review and Peer Evaluation meeting.

We look forward to your participation in the FY 2008 Annual Merit Review and Peer Evaluation meeting, which is presently scheduled for June 9-13, 2008 at the Marriott Crystal Gateway hotel in Arlington, VA.



JoAnn Milliken
DOE Hydrogen Program Manager
Office of Energy Efficiency and Renewable Energy

Hydrogen Production and Delivery:

Project #	Project Title, Performing Organization, PI	Final Wt. Score	New	Continue	Discontinue	Project Completed	Summary Comment
PD-01	*Low Cost Hydrogen Production Platform, Praxair, Tim Aaron*	3.24				X	Good focus on manufacturability and assembly. Reducing the cost and footprint of on-site hydrogen production is critical to reaching DOE goals. Additional data needed on hydrogen yield, generator durability, and space velocity. The research is viewed as needing to proceed to a demonstration phase.
PD-02	*Low-Cost Hydrogen Distributed Production Systems, H2Gen Inno. Inc., Frank Lomax*	3.41		X			Impressive accomplishment to complete 565 kg/day distributed natural gas platform. PSA developments will allow greater production flexibility. Lack of compression related work. Reviewers questioned whether ethanol testing would distract from primary objective (and asked to see more hydrogen generators built instead of directing the effort toward ethanol reforming) while also stating that funding H2Gen to research ethanol is a good idea. Partner roles unclear.
PD-03	*Integrated Hydrogen Production, Purification & Compression System, Linde, Satish Tamhankar*	3.06		X			Addresses fuel processor capital costs, O&M, and reliability and costs of hydrogen compression barriers by building an integrated membrane, fluidized bed reformer and metal hydride compressor system. Benefits of fluid bed reformer need to be clearly compared to conventional reforming technology. Process intensification will bring the cost down to DOE target levels.

Project #	Project Title, Performing Organization, PI	Final Wt. Score	New	Continue	Discontinue	Project Completed	Summary Comment
PD-04	*Bio-Derived Liquids Reforming, PNNL, Yong Wang*	2.86		X			Potential long term solution to distributed reforming system with very low Well to Wheels CO_2 emissions. Critical to the realization of renewable sources for hydrogen at the DOE targeted production cost of $3.00/gge by 2017. Strong early evaluation of catalyst performance for reforming of bio-derived fuels – an important topic as distributed reforming research transitions from natural gas to renewable feedstocks.
PD-05	*Biomass Gasification, GTI, Michael Roberts*	2.56	X	X			The reviewers recognized that it will be very challenging to find or develop a membrane system that will not foul in the biomass gasifier as proposed in this project. However, if successful, this project potentially offers substantial capital cost reduction and improved efficiency for biomass gasification which was deemed highly relevant to the Hydrogen Program. This project is just getting started. As recommended, experiments with the membrane(s) in the gasifier environment will be moved forward in the plan, and the project will be carefully reviewed for a Go/No-Go decision as soon as practical based on membrane(s) performance and a more thorough cost analysis of the this approach to biomass gasification.
PD-07	*Carbon Molecular Sieve Membrane as Reactor for Water Gas Shift Reaction, Media & Process Tech., Paul KT Liu*	3.27		X			Developing reactive separation membranes that do not use expensive materials (such as Pd-alloys) can have very significant payoff in overall hydrogen production costs. A membrane within the shift reactor will improve the CO conversion and reduce the shift reactor size. One reviewer disagreed that membrane reactors are critical in replacing conventional water gas shift however.

Project #	Project Title, Performing Organization, PI	Final Wt. Score	New	Continue	Discontinue	Project Completed	Summary Comment
PD-08	*Renewable Electrolysis Integrated System Development and Testing, NREL, Kevin Harrison*	3.13		X			The reviewers noted that hydrogen generation using renewable power was a very important part of the Hydrogen Initiative. They wanted to see more real world data which is in the plan. There was mixed comments on participation with industry- some of the reviewers indicated that there should be more participation and cost sharing from industry while others thought there was a great amount of industrial involvement already. Funding will continue on this project.
PD-09	*Biological Systems for Hydrogen Photoproduction, NREL, Maria Ghirardi*	3.46		X			The work is well aligned with the DOE technical targets and has made great progress considering its funding difficulties - the results could be far reaching and apply broadly to a variety of biological hydrogen production strategies. The scope should include milestones, decision points, down-select criteria, and an end date.
PD-10	*Photoelectrochemical Water Systems for H_2 Production, NREL, John Turner*	3.13		X			Good relevance and an important pathway to realize the DOE's long term objective of renewable hydrogen. The approach is appropriate to make progress toward the objectives. The work is open-ended, making it difficult to assess the degree to which this approach will contribute to the overall DOE objective of a technology readiness decision by 2015.

Project #	Project Title, Performing Organization, PI	Final Wt. Score	New	Continue	Discontinue	Project Completed	Summary Comment
PD-11	*Development of Solar-powered Thermochemical Production of Hydrogen from Water, UNLV, Chris Perkins*	3.38		X			This project had a very favorable review. The Earmark contract will come to an end in December, 2007. Effort on solar driven high temperature thermochemical water splitting cycles will be continued by the Hydrogen Program as appropriate. The plan in this area calls for a further down-selection of the potential cycles in FY08 from the current 7 to 1-3 for development as recommended by the reviewers.
PD-12	*Hydrogen Delivery Infrastructure Options Analysis, Nexant Inc., Bruce Kelly*	3.50		X			This project had a very favorable review. Significant progress has been made. The storage infrastructure needs and modeling will be reviewed by energy company logistics experts as recommended. This project will be completed during FY08.
PD-13	*Fundamental and Modeling of Pipeline Hydrogen Embrittlement, U of Illinois, Petros Sofronis*	3.48		X			This project had a very favorable review and will be continued. It was recognized for significant progress with limited funding. A good balance of theory and modeling with experimental data, and a strong interaction with stakeholders in industry and national labs.
PD-14	*FRP Hydrogen Pipeline, ORNL, Barton Smith*	3.23		X			This project had a favorable review. It was recognized that the use of fiber reinforced composite pipe has the potential for a capital cost breakthrough and elimination of hydrogen steel pipeline embrittlement concerns for a hydrogen pipeline infrastructure. As recommended, the plan for testing these composite pipeline structures will be carefully reviewed and augmented as appropriate by additional experts on composite and steel pipelines.

Project #	Project Title, Performing Organization, PI	Final Wt. Score	New	Continue	Discontinue	Project Completed	Summary Comment
PD-15	*Scale-up of Hydrogen Transport Membranes for IGCC and FutureGen Plants, Eltron Research Inc., Doug Jack*	3.26		X			This project had a favorable review and will be continued. The project was recognized for its relevance to the FutureGen project and Hydrogen Fuel Initiative. Additionally, the project is progressing to the next scale of development to further address critical issues. Some reviewers suggested that the timeline for development be accelerated.
PD-16	*Cost-Effective Method for Producing Self-Supporting Pd Alloy Membrane for Use in the Efficient Production of Coal-Derived Hydrogen, Southwest Research Institute, Kent Coulter*	3.33		X			Overall, this project had a favorable review. The initial phase of the project has been completed and the project team has been selected to continue work under a different solicitation. The team will continue to investigate its ultra-thin membrane technology and will continue to partner with the Colorado School of Mines in addition to Carnegie Mellon University and TDA Research.
PD-17	*Advanced Water Gas Shift Membrane Reactor, United Technologies, Suzanne Opalka*	3.10		X			This project scored an average review. The original contract of the project has been completed and the project is continuing under a new contract. The project team will undertake research, technology development, and economic analysis to further develop a sulfur-, halide-, and ammonia-resistant hydrogen-separation membrane. Based on alloys of palladium, copper, and transition metals, the membrane will potentially have commercially relevant hydrogen production flux and be capable of operating at high temperature and pressure.

Project #	Project Title, Performing Organization, PI	Final Wt. Score	New	Continue	Discontinue	Project Completed	Summary Comment
PD-18	*The Integration of a Structural Water Gas Shift Catalyst with a Vanadium Alloy Hydrogen Transport Device, Western Res. Ins. & U of Wyoming Res.Corp., Thomas Barton*	2.96				X	This project scored slightly below average and has been completed. The project had been successful in addressing some of the technical issues, particularly with brazing as a potential way for catalyst attachment. However, the outcome of tests on a working gasifier may highlight some of the potential issues.
PD-19	*High Flux Metallic Membranes for Hydrogen Recovery and Membrane Reactors, REB Research & Consulting, Robert Buxbaum*	3.18		X			This project scored favorably and was noted for its strong collaborative efforts and research partners. The project is continuing and will continue its membrane development efforts to address issues surrounding the flux, durability, and cost goals.
PD-20	*Sulfur-Iodine Thermochemical Cycle Laboratory-Scale Experiment, SNL/GA/CEA, Paul Pickard*	3.19		X			This project is one of the baseline technologies for the Nuclear Hydrogen Initiative. Overall comments were favorable, with emphasis recommended on resolving materials issues.
PD-21	*Hybrid Sulfur Thermochemical Process Development, SRS, Bill Summers*	2.97		X			Project is one of the baseline technologies for the Nuclear Hydrogen Initiative. Overall comments were favorable. Reviewer recommendations suggested more analysis on economic viability.
PD-22	*Laboratory-Scale High-Temperature Electrolysis System, INL/ANL/Ceramatec, Steve Herring*	3.24		X			The reviewers ranked this project as slightly above average. They generally approved of the step wise approach to achieve their goals. This is a long term, project and only the next year's plan was presented, which caused some of the reviewers to be concerned about the planning. The reviewers indicated that the SOEC durability was a potential road block. There should be significant development to improve the stack. This project will receive continued funding.

Project #	Project Title, Performing Organization, PI	Final Wt. Score	New	Continue	Discontinue	Project Completed	Summary Comment
PD-23	*Nuclear Reactor/Hydrogen Process Interface, INL, Steve Sherman*	3.22		X			This project scored very high on relevance but lower on accomplishments. Large number of collaborators was noted as both asset and weakness. Work is planned to continue with emphasis on actual heat exchanger testing, as well as continued modeling of reactor/process interactions.
PDP-01	*A Novel Slurry-Based Biomass Reforming Process, UTRC, Ying She*	2.88	X	X			The reviewers recognized that it may be very challenging for this biomass hydrolysis aqueous phase reforming approach to develop an effective catalyst that works well under the acidic conditions proposed and for this approach to match the favorable economics of standard biomass gasification. This project is just getting started. As recommended, the cost analysis task will be reviewed carefully including the assumptions concerning energy yields for the lignin stream. The plan focuses on the development of the catalyst as suggested by the reviewers. The plan will include a Go/No-Go decision as soon as is practical based on the cost analysis and catalyst development progress.
PDP-02	*Hydrogen from Water in a Novel Recombinant Oxygen-Tolerant Cyanobacteria System, Venter Institute, Qing Xu*	3.36		X			There was good progress on this project considering low level of government funding. Collaboration is good, but would benefit from more definitive check-points and cross-talk between the two research lines. The project represents a unique and attractive niche in the program.

Project #	Project Title, Performing Organization, PI	Final Wt. Score	New	Continue	Discontinue	Project Completed	Summary Comment
PDP-06	*Investigation of Bio-ethanol Steam Reforming over Cobalt Based Catalysts, Ohio State U, Umit Ozkan*	3.32		X			This project received very high marks for its relevance and approach to developing a precious metal-free catalytic system, however some reviewers also found the focus on data and experimentation excessive. The focus on acquiring a fundamental understanding of reaction networks and active sites was appreciated. Project publications were well received. The need for greater collaboration with partners was noted.
PDP-07	*Distributed Bio-Oil Reforming, NREL, Bob Evans*	3.13		X			NREL developed the atomizer, cracking process and autothermal bench scale reactor and validated the need for oxidation to increase CO production. Recent funding from Chevron demonstrates project merit as does a subcontract with University of Minnesota in systematic catalyst study. The need to expand catalytic results beyond methanol conversion was noted.
PDP-08	*Hydrogen Generation from Biomass-Derived Carbohydrates via Aqueous-Phase Reforming Process, Virent Energy Sys., Randy Cortright*	3.06		X			Novel technology. While some reviewers were very clear that the project could provide significant advancement of DOE goals, others were not. The proprietary approach was considered an impediment to scoring. Overall, the aqueous phase reforming technology was viewed as a critical process for producing hydrogen from renewable feedstocks. Appreciated principal investigator thorough response to prior year comments.

Project #	Project Title, Performing Organization, PI	Final Wt. Score	New	Continue	Discontinue	Project Completed	Summary Comment
PDP-09	*Integrated Short Contact Time Hydrogen Generator (SCPO), GE Global Res., Ke Liu*	3.12		X			Development of simplified reformers, particularly multi-fuel reformers viewed as a significant step towards meeting required DOE hydrogen cost targets (for the distributed production of natural gas). While some reviewers questioned the degree of innovation, others were very impressed with the novel science and engineering used to attack a difficult problem. Viewed as a model for industry, university, and national laboratory collaboration.
PDP-10	*Integrated Ceramic Membrane System for Hydrogen Production, Praxair, Joseph Schwartz*	2.67				X	Highly relevant for producing high purity hydrogen. Some reviewers noted differences in the research from project initiation to the conclusion questioning whether the hydrogen transport membrane research presented would result in a highly efficient, low cost hydrogen production platform (for the distributed production of natural gas).
PDP-11	*High-Performance, Durable, Palladium-Alloy Membrane for Hydrogen Separation & Purification, Pall Corp., Scott Hopkins*	3.21		X			While hydrogen permeance and separation factors meet or exceed DOE technical targets for metallic membranes, future testing of mixed gas streams (i.e. natural gas reformate) is important. Unclear how high hydrogen recovery will be achieved given low psi delta P tests. Future plans beyond durability, substrate and alloy testing were requested. Good team and work plan.
PDP-16	*Advanced Alkaline Electrolysis, GE Global Res., Richard Bourgeois*	3.16		X			This project received very high marks for its relevance and approach. The reviewers noted that a lot of progress has been made on the market analysis, but expected more to be accomplished on the technical side. The GE team is planning on building and demonstrating their units this year which will address many of the reviewer's comments. This project will continue.

Project #	Project Title, Performing Organization, PI	Final Wt. Score	New	Continue	Discontinue	Project Completed	Summary Comment
PDP-17	*EVermont Renewable Hydrogen Production and Transportation Fueling System, EVermont, Inc., Harold Garabedian*	2.66				X	This project had a below average review score. The reviewers noted that there were not a lot of significant technical accomplishments reported, that they were not using renewable energy, and that the work is not new as there are other refueling stations around the world.
PDP-19	*Hydrogen Regional Infrastructure Program in Pennsylvania, Concurrent Tech. Corp, David Moyer*	2.69		X			This project had a below average review score. The project covers several areas. Some were viewed favorably including the work on Pennsylvania and the Northeast I-95 Production and Delivery infrastructure analysis using the H2A models as well as the work on off-board storage vessels. Other areas such as sensors development, pipeline R&D and PSA purification enhancements were viewed as duplicative of other work in the program or being done by suppliers. This project will be continued to the complete expenditure of Congressionally Directed funding. DOE will continue to work with the contractor to modify the effort to maximize its value.
PDP-23	*Evaluation of Alternative Thermochemical Cycles, ANL, Michele Lewis*	2.93		X			Ongoing research; was noted for good collaboration with universities. Project should reach a major milestone of selecting an alternative cycle for development in coming year.
PDP-24	*UNLV High Temperature Heat Exchanger Development, UNLV, Tony Hechanova*	2.82		X			Actually 5 projects in one. Complexity of managing and adequately presenting such a wide range of topics was reflected in lower scores on project approach. Comments on apparent lack of focus are hoped to be resolved by renewed efforts to better align this project with NHI goals.

Project #	Project Title, Performing Organization, PI	Final Wt. Score	New	Continue	Discontinue	Project Completed	Summary Comment
PDP-26	*Test of High Temperature Electrolysis ILS Half Module, Ceramatec, Joe Hartvigsen*	3.23	X			X	The reviewers indicated that this project definitely supported the NHI and that it made solid contribution to its development. They indicated that there should be more development work in seals and materials to improve the stack durability. There were also recommendations that greater efforts in identifying suitable BOP components may result in better data (less interruptions due to component failures). This work continues under the core HTE project (PD-22).
PDP-28	*NHI Catalyst and Membrane Studies for Thermochemical Cycles at INL, INL, Dan Ginosar*	3.52		X			Highly relevant, highly scored project is important for improving economics and efficiency of thermochemical cycles being studied.
PDP-30	*Materials Issues and Experiments for HTE and SO_3 Electrolysis, ANL, David Carter*	3.48		X			This was a highly ranked project. The reviewers indicated that the approach was correct and that significant technical progress has been achieved in identifying the stack failure mechanisms. Understanding these mechanisms may make it easier to achieve a robust durable, long life SOEC stack. Funding will continue on this project.
PDP-31	*Corrosion Studies of Metallic Materials for Thermochemical Cycles, General Atomics, Bunsen Wong*	3.39			X		Project planned for discontinuance due to lower prioritization among thermochemical R&D.
PDP-32	*Membrane Development for Hybrid Sulfur Electrolysis and Oxygen Separation, SNL, Mike Hickner*	3.74		X			Extremely highly-scored project is vital to success of Hybrid Sulfur cycle development, as well as improving efficiency of Sulfur-Iodine cycle. Scores reflect breakthroughs being made and good collaboration with other researchers in this area.

Project #	Project Title, Performing Organization, PI	Final Wt. Score	New	Continue	Discontinue	Project Completed	Summary Comment
PDP-33	*Maximizing Light Utilization Efficiency & Hydrogen Production in Microalgal Cultures, UC Berkeley, Tasios Melis*	3.76		X			This highly scored project is very well aligned with the Program's R&D objectives for biological hydrogen production. Impressive progress has been made with limited funding.
PDP-36	*Photoelectrochemical Generation of Hydrogen Using Sonicated Hybrid Titania Nanotube Arrays, U of Nev. Reno, Mano Misra*	2.70		X			Considering the external bias requirements for effective photocurrent levels in this TiO_2 work, and the lack of a clear pathway for achieving the longer-term DOE photocurrent and STH efficiency goals with this material system, this work did not adequately address the DOE RD&D objectives for un-assisted PEC solar water splitting. It is difficult to differentiate from conventional TiO_2, which is known not to work – not clear how/why nanotubes are an improvement.
PDP-37	*Photoelectrochemical Hydrogen Production: UNLV-SHGR Program Subtask, UNLV, Eric Miller*	3.37		X			This project represents a great cross-university/ industry/national lab collaboration covering multiple topics that is clearly working toward DOE's PEC targets. A benefit of this approach will be the development of theoretical tools that will help all participants and periodic (quarterly) group feedback can accelerate attainment of R&D goals.
PDP-40	*Adapting Planar Solid Oxide Fuel Cells for Distributed Power Generation, Ohio University, Andres Marquez*	2.34		X			This project was rated very low. The reviewers noted that it seemed more aligned to the SECA program than to the Hydrogen Initiative. The reviewers noted that progress had been made in identifying contaminant concerns. However, they noted that progress seemed to be slow, that the integrated concept was not thought out very well, and that plans for future work need to be made. We will work with the researchers to increase their work on hydrogen production technologies.

Project #	Project Title, Performing Organization, PI	Final Wt. Score	New	Continue	Discontinue	Project Completed	Summary Comment
PDP-42	*Ohio Distributed Hydrogen Project, Ohio University, David Bayless*	2.33		X			This project was rated very low. The reviewers noted that hydrogen production was one aspect of the work, but not the primary objective of the project. It seemed more focused on stationary power generation using coal and SOFC than hydrogen production. The reviewers thought the researcher covered too many areas, and that it should be more focused. This was reflected in their observations that technical progress has been slow. There were many recommendations the project scope be more focused on one or two areas, and one recommendation that funding be discontinued. We will work with the researchers to refine their scope.

Hydrogen Storage:

Project #	Project Title, Performing Organization, PI	Final Wt. Score	New	Continue	Discontinue	Project Completed	Summary Comment
ST-01	*DOE Hydrogen Sorption CoE Overview, NREL, Mike Heben*	2.82		X			The HSCoE should incorporate down select decisions regularly to ensure that R&D stresses storage of hydrogen near ambient temperature and moderate pressure. Increase collaborations internally and externally to leverage resources.
ST-02	*NREL Research as part of Hydrogen Sorption CoE, NREL, Anne Dillon*	3.07		X			Increased experimental emphasis was recognized. Continue to emphasize synthesis of materials with improved binding energy and volumetric and gravimetric capacity.

Project #	Project Title, Performing Organization, PI	Final Wt. Score	New	Continue	Discontinue	Project Completed	Summary Comment
ST-03	*Hydrogen Storage by Spillover, U of Michigan, Ralph Yang*	2.87		X			Increase collaborations to improve understanding of spillover mechanisms and to improve reproducibility of synthesis and performance of materials.
ST-04	*Theoretical Models of H_2-SWNT Systems for Hydrogen Storage and Optimization of SWNT Production, Rice U, Boris Yakobson*	3.16		X			Increase emphasis on understanding spillover and implications for materials synthesis. For material synthesis, stress optimizing binding energy while maintaining or increasing capacity.
ST-05	*Cloning Single Wall Carbon Nanotubes for Hydrogen Storage, Rice U, Jim Tour*	3.00		X			Emphasize property testing (capacity, binding energy, kinetics). Scaffold work is promising. Continue to emphasize higher temperature storage.
ST-06	*Metal-doped Carbon Aerogels for Hydrogen Storage, LLNL, Ted Baumann*	2.96		X			Emphasize understanding on whether metal doped C-aerogels are promising for near ambient storage. Continue collaborations with MHCoE for aerogel as a scaffold material.
ST-07	*Enabling Discovery of Materials With A Higher Heat of H_2 Adsorption, Air Products, Alan Cooper*	3.04		X			Stress synthesis of F-N nanoporous materials. Confirm predictions made on spillover materials (validate theory through experiments). Increase strategic leadership role in HSCoE.
ST-08	*Advanced Boron and Metal Loaded High Porosity Carbons, Penn State, Mike Chung*	2.97		X			Leverage resources on the most promising synthesis approaches. Widen the range of dopants explored. Clarify whether B-level achieved is reaching the limit and whether B-incorporation is increasing binding energy sufficiently.
ST-09	*Carbide-Derived Carbons with Tunable Porosity Optimized for Hydrogen Storage, U of Penn./Drexel Univ., Jack Fischer*	3.14		X			Emphasize material design towards non-cryogenic operation. Surface chemical modification results (to increase binding) look promising. Approaches to increase volumetric capacity appear promising.

Project #	Project Title, Performing Organization, PI	Final Wt. Score	New	Continue	Discontinue	Project Completed	Summary Comment
ST-10	*Hydrogen Storage in Metal-Organic Frameworks, UCLA, Omar Yaghi*	3.42		X			Stress reticular and/or hybrid structures for storage towards ambient temperature. Working on frameworks with higher hydrogen binding energies seems to be essential. Currently the best in class for cryogenic storage materials.
ST-14	*DOE Metal Hydride CoE Overview, SNL, Lennie Klebanoff*	2.86		X			The MHCOE should formulate comprehensive down-select criteria and apply them regularly to their research areas. Improvement of kinetics needs more emphasis. The theoretical capabilities of the center should be better focused and utilized throughout all research areas of the center.
ST-15	*Sandia Research as part of the Metal Hydride CoE, SNL, Ewa Ronnebro*	3.26		X			Focus on lower temperature systems. Use the combinatorial approach to more rapidly screen systems for potential candidates and to search for catalysts to address kinetic barriers. The theoretical effort should continue to be used to guide the experimental effort.
ST-16	*Lightweight Intermetallics for Hydrogen Storage, General Electric, J.C. Zhao*	3.00		X			Greater emphasis is needed on criteria other than just weight capacity. Efforts should be made to identify catalysts to improve kinetics. Criteria for the go/no go decision on $Mg(BH_4)_2$ need to be formulated and applied. More collaborations are encouraged.
ST-17	*First-Principles Modeling of Hydrogen Storage in Metal Hydride Systems, Univ. of Pittsburgh, Karl Johnson*	2.96		X			Theoretical predictions are useful for improving the efficiency of experimental efforts, however closer collaboration with experimentalists is encouraged in all research areas of the center. The methodology needs to include consideration of reaction pathways and not just the predicted lowest energy reaction products.

Project #	Project Title, Performing Organization, PI	Final Wt. Score	New	Continue	Discontinue	Project Completed	Summary Comment
ST-18	*Thermodynamically Tuned Nanophase Materials for Reversible Hydrogen Storage, HRL Laboratories, Ping Liu*	3.27		X			The overall approach and work effort was found appropriate. Incorporation of materials other than just Mg is encouraged.
ST-20	*Synthesis and Characterization of Alanes for Automotive Applications, BNL, Jason Graetz*	2.98		X			The alane project was considered extremely relevant and the use of organic adducts praised. Focus future work on regeneration processes and energetics of regeneration.
ST-21	*Chemical Vapor Synthesis of Nanocrystalline Binary and Complex Metal Hydrides for Hydrogen Storage - Understanding and Discovery of H_2 Storage Materials Involving Metal Amides, Univ. of Utah, Zak Fang*	2.82		X			The quantification of NH_3 desorbed from the amide systems needs to be a top priority. Consider a go/no go decision if the NH_3 concentration is found to be too high. The determination of reaction mechanisms should also be of higher priority.
ST-22	*Fundamental Safety Testing and Analysis of Hydrogen Storage Materials & Systems, SRNL, Don Anton*	3.06		X			This project was considered to be very important for the program as a whole, however there was a concern that results may be used to preclude R&D of materials that might be of value. The test plans should be expanded to be more applicable to on-board applications versus materials transport.
ST-23	*Hydrogen Storage by Reversible Hydrogenation of Liquid-phase Hydrogen Carriers, Air Products, Alan Cooper*	2.97		X			Continue to pursue material with high capacity, lower release temperature and efficient & inexpensive catalyst while taking the system analysis results of ST-31 into consideration.
ST-24	*DOE Chemical Hydrogen CoE Overview, LANL, Bill Tumas*	3.59		X			Apply up-front system analysis (e.g. R&H analysis) to identify show stoppers and guide material development. Pursue new promising materials including non-boron materials. Pursue high throughput approach (including catalyst discovery) to accelerate both hydrogen release and ammonia regeneration approaches.

Project #	Project Title, Performing Organization, PI	Final Wt. Score	New	Continue	Discontinue	Project Completed	Summary Comment
ST-25	*Novel Approaches to Hydrogen Storage: Conversion of Borates to Boron Hydrides, Rohm and Haas, Suzanne Linehan*	3.28		X			Complete experimental work and calculate sodium borohydride regeneration efficiency as well as cost-include consideration of forecourt operation and return of spent fuel.
ST-26	*Electrochemical Hydrogen Storage Systems, Penn State, Digby Macdonald*	2.91		X			Complete experimental work and present data for sodium borohydride go/no-go decision review. Include energy efficiency and cost analyses.
ST-27	*Amineborane Hydrogen Storage, U of Penn., Larry Sneddon*	3.67		X			Continue to develop and optimize additives to improve capacity and release rates (especially for release of the second equivalent of hydrogen). Increase emphasis on efficient and economic spent fuel regeneration.
ST-28	*PNNL Research as part of the Chemical Hydrogen CoE, PNNL, Chris Aardahl*	3.50		X			Increase emphasis on identifying better digestion process for efficient regeneration of ammonia borane. Improve hydrogen release kinetics (especially for release of the second equivalent of hydrogen) as well as capacity. Investigate and identify path forward for the scaffold work.
ST-29	*LANL Research as part of the Chemical Hydrogen CoE, LANL, Tom Baker*	3.35		X			Place focused effort on efficient catalyst screening and development to meet hydrogen release kinetics and capacity needs. Transform homogeneous catalyst for heterogeneous catalyst applications. Narrow down regeneration options expeditiously and further develop promising approaches. Conduct up-front engineering studies to identify show stoppers early and guide material development to address critical material development issues.
ST-30	*Main Group Element and Organic Chemistry for Hydrogen Storage and Activation, U of Alabama, David Dixon*	3.39		X			Compare experimental and computational data and confirm/adjust the gas phase computational model as appropriate. Focus experimental work on material with promising capacity taking system requirements into consideration.

Project #	Project Title, Performing Organization, PI	Final Wt. Score	New	Continue	Discontinue	Project Completed	Summary Comment
ST-31	*System Level Analysis of Hydrogen Storage Options, ANL, Rajesh Ahluwalia*	3.34		X			Continue sensitivity analyses for current designs to assess potential design parameters for future systems. Cross-check underlying assumptions with other stakeholders.
ST-32	*Analyses of Hydrogen Storage Materials and On-Board Systems, TIAX, Stephen Lasher*	3.43		X			Periodically revisit estimates made in previous years, work with industry to check validity of original assumptions and update as required. Must also stay current with progress made outside DOE portfolio.
ST-33	*International Standardized Testing Protocols for Hydrogen Storage Materials, NREL/HyEnergy, Karl Gross*	2.95		X			Consider addressing sample handling conditions and respective protocols and integrate feedback from experts. Coordinate with SwRI standardized testing facility and publicize documentation widely.
STP-02	*Conducting Polymers as New Materials for Hydrogen Storage, U of Penn., Pen-Cheng Wang*	2.62			X		This project is discontinued- PI recently deceased. This is a promising avenue of research for sorbent materials; DOE is exploring options to continue similar work elsewhere within its portfolio.
STP-03	*Characterization of Hydrogen Adsorption by NMR, U of North Carolina, Yue Wu*	3.45		X			This project has an important characterization role in the HSCoE. Extend study to spillover materials, advanced MOFs, and SWNT networks.
STP-04	*Synthesis of Small Diameter Carbon Nanotubes and Microporous Carbon Materials for Hydrogen Storage, Duke U, Jie Liu*	3.04		X			The shift from small diameter nanotubes towards microporous carbon materials is recommended. Coordination is needed to avoid unnecessary duplication.
STP-06	*Single Walled Carbon Nanohorns for Hydrogen Storage and Catalyst Supports, ORNL, David Geohegan*	2.75		X			Need to demonstrate/ assess that the nanostructured materials under study have the potential to reach room temperature storage at moderate pressure.
STP-07	*Enhanced Hydrogen Dipole Physisorption, CalTech, Channing Ahn*	2.73		X			The characterization capabilities of this group are key to the HSCoE. Effort should be increased on new material syntheses. Collaborations should be increased as appropriate.

Project #	Project Title, Performing Organization, PI	Final Wt. Score	New	Continue	Discontinue	Project Completed	Summary Comment
STP-10	*Solutions for Chemical Hydrogen Storage: Hydrogenation/ Dehydrogenation of B-N Bonds, U of Washington, Karen Goldberg*	3.26		X			Improve hydrogen release for the catalyst with fast kinetics. Continue to develop non-precious metal catalyst while addressing selectivity, efficiency and capacity issues. Investigate if there is a hydrogen purity issue related to the organic linker of the catalyst.
STP-11	*Chemical Hydrogen Storage Using Polyhedral Borane Anion Salts, UMO, Fred Hawthorne*	2.42		X			Need to improve both hydrogen release kinetics and capacity. Continue to identify non-precious metal catalysts. Increase communication and collaboration with center partners working on sodium borohydride regeneration- this work is tied to the sodium borohydride go/no-go decision since spent fuel regeneration also involves conversion of B-O to B-H.
STP-12	*Development of Advanced Chemical Hydrogen Storage and Generation System, Millennium Cell, Oscar Moreno*	3.03		X			Complete storage system and cost analysis for the modeled design to meet the sodium borohydride go/no-go decision schedule.
STP-13	*Combinatorial Synthesis and High Throughput Screening of Effective Catalysts for Chemical Hydrides, Intematix, Jonathan Melman*	2.79		X			Provide more data and detail of work done, including catalyst library selection rationale.
STP-14	*Chemical Hydrogen Storage using Ultra-High Surface Area Main Group Elements, UC Davis, Susan Kauzlarich*	2.71		X			Determine viability of the high surface area material under investigation soon. Continue support to the Chemical Hydrogen Storage Center partners for ammonia borane regeneration.
STP-17	*Hydrogen Fuel Cells and Storage Technology Project at UNLV, UNLV, Clemens Heske*	2.07		X			Candidate materials should be identified and tested for hydrogen storage capacity as soon as possible. There is concern that this project will produce an in-depth investigation of materials and processes that aren't particularly relevant to the overall DOE hydrogen storage program.

Project #	Project Title, Performing Organization, PI	Final Wt. Score	New	Continue	Discontinue	Project Completed	Summary Comment
STP-24	*Complex Hydrides for Hydrogen Storage Studies of the $Al(BH_4)_3$ System, ORNL, Gilbert Brown*	2.92		X			While the investigation of unique high weight capacity borohydrides is of interest, a go/no go decision on these types of materials should be made within a year or so. Consideration should be given to the toxicity of B_2H_6 and other volatile species and their elimination from the desorbed H_2.
STP-25	*High Throughput Combinatorial Chemistry Development of Complex Hydrides, Intematix, Darshan Kundaliya*	3.05		X			While high-throughput methods are important to rapidly screen many materials/reactions, there is a need to develop a better data mining technique. There is concern regarding the validity of the detection method. Stronger collaboration with center partners is encouraged.
STP-26	*Thermodynamically Tuned Nanophase Materials for Reversible Hydrogen Storage: Structure & Kinetics of Nanoparticle and Model System Materials, Stanford U, Bruce Clemens*	2.92		X			Expand research focus beyond Mg thin films to materials more relevant to the center. The relevance of thin film reactions to bulk materials needs to be demonstrated. The results of the study need to be communicated with the theory group for inclusion into their models.
STP-27	*Alane Electrochemical Recharging, SRNL, Ragaiy Zidan*	3.12		X			Characterize products. The use of non-aqueous electrolyte was considered a major advancement of the project, however yield, efficiency and energy intensity of the process needs consideration.
STP-28	*Synthesis of Nanophase Materials for Thermodynamically Tuned Reversible Hydrogen Storage, California Institute of Tech, Channing Ahn*	2.71		X			When experimental results do not agree with the theoretical predictions, it is important to feed information back to the theory groups for refinement of their models. The work scope appears very aggressive and may need refinement to better meet the needs of the CoE.

Project #	Project Title, Performing Organization, PI	Final Wt. Score	New	Continue	Discontinue	Project Completed	Summary Comment
STP-29	*Effect of Trace Elements on Long-Term Cycling and Aging Properties of Complex Hydrides for Hydrogen Storage, U of Nevada, Reno, Dhanesh Chandra*	3.35		X			The studies should be more focused on material cycling and impurity effects. Closer integration with the theory group is encouraged.
STP-31	*Metal Hydride-Based Hydrogen Storage, U of Illinois, Ian Robertson*	3.23		X			Expand collaborations beyond the MHCoE. The experimental efforts should also be expanded to include the impact of impurity and oxidation reactions on hydrogenation/dehydrogenation and in situ studies of microstructural changes during hydrogenation/dehydrogenation reactions of complex hydrides.

Fuel Cells:

Project #	Project Title, Performing Organization, PI	Final Wt. Score	New	Continue	Discontinue	Project Completed	Summary Comment
FC-01	*Fuel Cell Systems Analysis, ANL, Rajesh Ahluwalia*	2.91		X			Prioritize impurity modeling. System model should be used. Focus on transient designs/off-design points.
FC-02	*Neutron Imaging Study of the Water Transport in Operating Fuel Cells, NIST, David Jacobson*	3.67		X			Take "snapshots" during freezing process. An additional project to investigate transient phenomena during startup, shutdown, and load-following would be beneficial. Three-dimensional effects are likely to be important.
FC-03	*Microstructural Characterization of PEM Fuel Cell MEAs, ORNL, Karren More*	3.42		X			Should include different cell locations in examinations of used samples. Sub-surface characterization needs to be addressed. Need to characterize changes in carbon support.

Project #	Project Title, Performing Organization, PI	Final Wt. Score	New	Continue	Discontinue	Project Completed	Summary Comment
FC-04	*Novel Approach to Non-Precious Metal Catalysts, 3M, Radoslav Atanasoski*	3.13				X	Progress is significant. Not only relevant to this 3M project, efforts represent a potential high pay-off option in oxygen electrocatalysis.
FC-05	*Novel Non-Precious Metals for PEMFC: Catalyst Selection Through Molecular Modeling and Durability Studies, U of So. Carolina, Branko N. Popov*	2.97				X	Catalyst layers are too thick for reasonable conductivity. PI should run DOE-specified durability tests (as opposed to steady-state low potential tests).
FC-06	*Development of Transition Metal/Chalcogen Based Cathode Catalysts for PEM Fuel Cells, Ballard, Stephen Campbell*	2.77			X		Show results in terms of activity per site and site density (sites/cm^3). Product of these two is A/cm^3 and the target should be 130 A/cm^3.
FC-07	*Applied Science for Electrode Performance, Cost, and Durability, LANL, Bryan Pivovar*	2.79		X			Use higher wt % of Pt (or Pt alloy) on C. Look at effect on durability. Pursue sensitivity measurements to identify factors that affect fuel cell failure before focusing on specific factors. The bonding of electrodes to the membrane should be considered for the project scope.
FC-08	*Development of Polybenzimidazole-based High Temperature Membrane and Electrode Assemblies for Stationary Applications, Plug Power, John Vogel*	3.22				X	Cost predictions for MEA and system are vital – if predictions cannot achieve target values, the need of this program decreases significantly. Excellent work.
FC-09	*Development of a Low-cost, Durable Membrane and MEA for Stationary and Mobile Fuel Cell Applications, Arkema Chemicals, Jung Yi*	3.02				X	Follow-on projects should report more structural characterization, particularly as a function of time in these systems. Lifetime data needs to be presented from fuel cell tests.
FC-10	*MEA and Stack Durability for PEM Fuel Cells, 3M, Mike Yandrasits*	3.17				X	Need to develop in more detail the relationship of materials chemistry to failure modes and lifetime prediction.

Project #	Project Title, Performing Organization, PI	Final Wt. Score	New	Continue	Discontinue	Project Completed	Summary Comment
FC-11	*Improved Membrane Materials for PEM Fuel Cell Applications, U of So. Mississippi, Robert Moore*	2.97		X			Compare current approach to the literature. Ensure that enhanced performance is not due to thickness reduction of the membrane. It would be good to use gel permeation chromatography or another analytical technique to verify the theory that the MW is decreasing with degradation due to loss of small fragments.
FC-12	*Poly(p-phenylene Sulfonic Acid)s with Frozen-in Free Volume for Use in High Temperature Fuel Cells, Case Western Reserve University, Morton Litt*	2.95		X			Measure conductivity in the transverse direction. Involve industry partner to comment on manufacturability and cost. Measure through-plane conductivity. It may not be productive to focus on materials that do not yield films. At a minimum, some degradation studies need to be performed on candidate materials.
FC-13	*Poly(cyclohexadiene)-Based Polymer Electrolyte Membranes for Fuel Cell Applications, U of Tennessee, Jimmy Mays*	2.67		X			Explore block chemistry further. Develop monomers with protected sulfonic acid groups to avoid post-sulfonation. Reduce sol-gel chemistry effort. Eliminate crosslinking for at least baselining purposes. Optimize proton conductivity and improve mechanicals later.
FC-14	*NanoCapillary Network Proton Conducting Membranes for High Temperature Hydrogen/Air Fuel Cells, Case Western Reserve University, Peter Pintauro*	2.83		X			Carry out detailed study of active fiber loading in inert matrix to determine conductivity, power, uptake, and stability. Durability and low RH studies to be added.
FC-15	*Lead Research and Development Activity for High Temperature, Low Relative Humidity Membrane Program, U of Central Florida, James Fenton*	3.01		X			Run durability tests on membranes with and without phosphotungstic acid. May be appropriate to set up a "support lab" for conductivity measurements.

Project #	Project Title, Performing Organization, PI	Final Wt. Score	New	Continue	Discontinue	Project Completed	Summary Comment
FC-16	*Protic Salt Polymer Membranes: High-Temperature Water-Free Proton-Conducting Membranes, Arizona State, Dominic Gervasio*	3.05		X			Add evaluation of these protic ionic liquids as catalyst ionomers. Morphology studies are needed for the stable protic salt membranes.
FC-17	*Novel Approaches to Immobilized Heteropoly Acid (HPA) Systems for High Temperature, Low Relative Humidity Polymer-Type Membranes, Colorado School of Mines, Andrew Herring*	3.35		X			Upon blending with polymer "X", significant testing will be necessary to prove this particular concept for the "Go/No-Go" decision. Emphasize low RH conductivity (< 70% RH).
FC-18	*High Temperature Membrane with Humidification-Independent Cluster Structure, FuelCell Energy, Inc., Ludwig Lipp*	3.03		X			Testing that assures stability of the additives in the membrane should be done next year. Obtain *in situ* mechanical cycling protocol from FreedomCAR Fuel Cell Tech Team.
FC-19	*Design and Development of High-Performance Polymer Fuel Cell Membranes, General Electric, Ryo Tamaki*	2.69		X			Develop proper collaborator to identify membrane/electrode interface properties and for fuel cell testing.
FC-20	*Fluoroalkylphosphonic-acid-based Proton Conductors, Clemson, Stephen Creager*	3.39		X			Prepare membranes using the "best" electrolytes for test and evaluation. Select alternative monomer with endgroups compatible with aqueous polymerization.
FC-21	*Dimensionally Stable High Temperature Membranes, Giner, Cortney Mittelsteadt*	3.26		X			The laser drilled 2-D support is impractical and should be used to direct research using the 3D support. Balance the need to understand the poor fuel cell performance against the need to develop new ionomers with low equivalent weight.
FC-22	*New Proton Conductive Composite Materials with Co-continuous Phases Using Functionalized and Crosslinkable TFE/VDF Fluoropolymers, Penn State, Serguei Lvov*	3.08		X			Reduce the number of additive options. The project could benefit from theory/simulation of the conduction mechanism to see how it matches with experiment.

Project #	Project Title, Performing Organization, PI	Final Wt. Score	New	Continue	Discontinue	Project Completed	Summary Comment
FC-23	*Advanced Materials for Proton Exchange Membranes, Virginia Tech, James McGrath*	3.35		X			Consider doing cost of production study of most promising membranes.
FC-25	*Center for Intelligent Fuel Cell Materials Design Phase 1, Chemsultants International, Denise Katona*	1.72		X			Emphasize investigations of composite membranes and conductivity testing. Add a sound cost analysis. Evaluate membrane stability. Focus on membrane materials characterization.
FC-26	*Economic Analysis of Polymer Electrolyte Membrane Fuel Cell Systems, Battelle, Kathya Mahadevan*	3.31		X			A more detailed but much broader project in the future that focuses on 2-3 very specific market segments like fork trucks and telecom backup power is desirable.
FC-27	*Direct Hydrogen PEMFC Manufacturing Cost Estimation for Automotive Applications, TIAX, Stephen Lasher*	3.34		X			Stack conditioning should be covered in the stack assembly section.
FC-28	*Mass Production Cost Estimation for Direct H_2 PEM Fuel Cell System for Automotive Applications, DTI, Brian James*	3.49		X			Components from a working stack should be considered for the study to reflect the actual manufacturing cost. Evaluate alternative catalyst.
FC-29	*Platinum Recycling Technology Development, Ion Power, Inc., Stephen Grot*	3.13		X			Complete a preliminary economic analysis of the proposed project. Investigate how recovery process must be developed for a unitized assembly including seals, gaskets, adhesives, etc. Work on alloy recycling.
FC-30	*Platinum Group Metal Recycling Technology Development, BASF, Larry Shore*	3.23		X			Complete the economic analysis and prototype process demonstration. Quantify CO_2 emissions from energy usage.
FCP-01	*Component Benchmarking, LANL, Tommy Rockward*	3.07		X			Carry out statistical analysis of durability test results. Recommend putting significant resources and timeline commitments on the impurities work.
FCP-04	*Kettering University Fuel Cell Project, Kettering University, Joel Berry*	2.77		X			Focus work on overcoming key barriers.

Project #	Project Title, Performing Organization, PI	Final Wt. Score	New	Continue	Discontinue	Project Completed	Summary Comment
FCP-08	*University of South Carolina Fuel Cell Design Project, U of So. Carolina, John Van Zee*	2.62		X			Focus on performance and diagnostics rather than modeling. Program should compare PBI fuel cell to a phosphoric acid fuel cell that uses a silicon carbide for matrix.
FCP-09	*Development of a 5 kW Prototype Coal-based Fuel Cell, University of Akron, Steven Chuang*	2.55		X			Suggest system design and efficiency analysis.

Technology Validation:

Project #	Project Title, Performing Organization, PI	Final Wt. Score	New	Continue	Discontinue	Project Completed	Summary Comment
TV-01	*Controlled Hydrogen Fleet and Infrastructure Demonstration and Validation Project, DaimlerChrysler, Klaus BonHoff*	3.46		X			An excellent match with DOE targets and the President's objectives. The project is important effort to demonstrate the feasibility of fuel cell vehicles and hydrogen infrastructure.
TV-02	*Hydrogen Fuel Cell Vehicle & Infrastructure Demonstration Program Review, Ford, Greg Frenette*	3.42		X			An excellent match with the DOE targets and the President's objectives. The project is important effort to demonstrate the feasibility of fuel cell vehicles and hydrogen infrastructure.
TV-03	*Controlled Hydrogen Fleet and Infrastructure Demonstration and Validation Project, Chevron, Dan Casey*	3.28		X			An excellent match with the DOE targets and the President's objectives. The project is important effort to demonstrate the feasibility of fuel cell vehicles and hydrogen infrastructure.
TV-04	*Hydrogen Vehicle and Infrastructure Demonstration and Validation, General Motors, Roz Sell*	3.39		X			An excellent match with the DOE targets and the President's objectives. The project is important effort to demonstrate the feasibility of fuel cell vehicles and hydrogen infrastructure.

Project #	Project Title, Performing Organization, PI	Final Wt. Score	New	Continue	Discontinue	Project Completed	Summary Comment
TV-05	*Controlled Hydrogen Fleet & Infrastructure Analysis, NREL, Keith Wipke*	3.76		X			Critical effort to collect, organize and distribute the fuel cell vehicle and infrastructure data.
TV-06	*Validation of an Integrated Hydrogen Energy Station, Air Products, Dan Tyndall*	3.29		X			Potential to fill real-world data needs for energy stations and bio-waste energy hydrogen production.
TV-07	*California Hydrogen Infrastructure Project, Air Products, Ed Heydorn*	3.54		X			Validation of the technology is on the critical path to establishing a hydrogen energy structure in the US.
TV-08	*Cryogenic Capable Pressure Vessels for Vehicular Hydrogen Storage, LLNL, Salvador Aceves*	3.26		X			Strong relevance to DOE targets for storage volume and weight
TV-10	*Technology Validation: Fuel Cell Bus Evaluations, NREL, Leslie Eudy*	3.67		X			Excellent collaboration with transit companies and international partners, reporting of results and dissemination.
TVP-02	*Geographically Based Hydrogen Infrastructure Scenario Analysis, NREL, Margo Melendez*	3.29				X	Any additional funding will be from Systems Analysis.
TVP-04	*Policy Options for Hydrogen Vehicles and Infrastructure, TIAX, Stefan Unnasch*	3.28				X	Any additional funding will be from Systems Analysis
TVP-08	*Hydrogen Filling Station, UNLV, Rick Hurt and Yitung Chen*	3.11		X			UNLV needs to get some hydrogen consumption to match their production capacity
TVP-11	*Florida Hydrogen Initiative, Florida Hydrogen Initiative, Ed Levine*	2.91		X			This is 3 unrelated projects with some more relevant than others. Distinctions need to be clearer.

Safety Codes and Standards:

Project #	Project Title, Performing Organization, PI	Final Wt. Score	New	Continue	Discontinue	Project Completed	Summary Comment
SA-01	*Codes, Standards and Permitting Materials, NREL, Jim Ohi*	2.99		X			This project is well-organized with broad participation from domestic and international codes and standards development organizations. This project will continue to produce significant results toward the development of a comprehensive and performance-based set of codes and standards for the safe use of hydrogen. This project has also produced significant contributions from a collaborative effort between Energy providers and the Fire Safety and Building Code community to develop and implement tools for the permitting of hydrogen refueling stations.
SA-02	*Hydrogen Materials R&D, SNL, Brian Somerday*	3.55		X			A Technical Reference Manual of experimental data on hydrogen materials compatibility has been developed to ensure that scientifically sound data are available for the codes and standards development process. This effort will expand to investigate the effects of hydrogen on non-metal materials.
SA-03	*H_2 Incident Reporting Database and H_2 Safety Best Practices Website, PNNL, Linda Fassbender*	3.17		X			This project consists of establishing a web-based system for open sharing of lessons learned from hydrogen incidents and near misses and developing a Hydrogen Best Practices database to share the knowledge and experience already attained in industry, aerospace, and elsewhere.

Project #	Project Title, Performing Organization, PI	Final Wt. Score	New	Continue	Discontinue	Project Completed	Summary Comment
SA-04	*Hydrogen Quality, NREL/LANL, Jim Ohi*	3.39		X			This project is developing experimental data on the effects of hydrogen contaminants on fuel cell performance. This project brings a team with strong modeling capabilities, including ANL, LANL, HNEI, Univ. Connecticut, Univ. of South Carolina, Ballard, and NREL. The data from this project and the modeling capabilities of its participants will be leveraged internationally to develop an ISO standard for hydrogen quality.
SA-06	*Hydrogen Safety Panel, PNNL, Steven Weiner*	3.53		X			This project helps ensure the safety of DOE-funded projects and brings expertise from industry, academia, government and the private sector to conduct safety reviews and to make safety recommendations.
SAP-02	*Hydrogen Safety Sensors, Intelligent Optical Systems, Bob Lieberman*	2.68			X		This project aims to develop hydrogen safety sensors based on fiber optic technology. This project was not competitively selected and will not be funded in FY 2008.

Education:

Project #	Project Title, Performing Organization, PI	Final Wt. Score	New	Continued	Discontinued	Project Completed	Summary Comment
ED-01	*Hydrogen Technology and Energy Curriculum (HyTEC), Schatz Energy Research Center, Jim Zoellick*	3.13		X			Aligns well with overall DOE hydrogen education targets; completed a significant amount of work despite limited DOE funding; strong partnerships for real-life demonstration and distribution of classroom materials. Continue, pending FY08 appropriations.
ED-02	*H_2 Educate!, NEED, Rebecca Lamb*	3.45		X			Well linked to address education barriers; strong network and partnerships have worked to achieve great success despite limited DOE funding. Continue, pending FY08 appropriations.
ED-03	*First Responder Education, PNNL, Marylynn Placet*	3.38		X			Long overdue effort; well tested prior to launch, strong approach with review and partnerships, good distribution; good success to date; prop-based training for future will help fill a need, consider certification. Continue, pending FY08 appropriations.
ED-04	*Increasing "H2IQ": A Public Information Program, The Media Network, Henry Gentenaar*	3.21		X			Important outreach effort, although a daunting task; well-defined, flexible approach; focus on metrics to determine effectiveness. Continue, pending FY08 appropriations.

Analysis:

Project No.	Project Title, Performing Organization, PI	Final Score	New	Continued	Discontinued	Project Completed	Summary Comment
AN-01	*Hydrogen Production Infrastructure Options Analysis, Directed Techs., Brian D. James*	3.29				X	The model has been completed, peer reviewed, and available for analysis applications. The model provides an optimized infrastructure build out to meet hydrogen demand. Potential project additions may be to incorporate risk analysis and linkage to the Macro-System Model.
AN-02	*Impact of Hydrogen Production on U.S. Energy Markets, EEA, Harry Vidas*	2.84		X			Incorporation of new technologies, resources, and carbon capture and sequestration strengthens the national MARKAL model's representation and modeling of hydrogen with other fuels. More analysis of policy and impact of government decisions should be provided.
AN-03	*Analysis of the Hydrogen Production and Delivery Infrastructure as a Complex Adaptive System, RCF, Inc., George Tolley*	2.80		X			Model provides a novel approach to understanding uncertainty and consumer choice for a hydrogen system and rollout scenarios in non-optimal analysis. The model is complex and not very transparent. The model and assumptions need to be clear and peer reviewed.
AN-04	*HyDRA - Resource Analysis, NREL, Johanna Levene*	3.37		X			Mapping resource supply to demand based on a Geographic Information System (GIS) is a strong tool. Provides valuable information in a visual format for decision makers. The model and analysis is in the early phases of development.
AN-05	*Macro-System Model, NREL, Mark Ruth*	3.52		X			Providing analysis and modeling of production, delivery and emissions provides for consistency of assumptions and results. Project will critical for R&D and planning decisions. Good work.

Project No.	Project Title, Performing Organization, PI	Final Score	New	Continued	Discontinued	Project Completed	Summary Comment
AN-06	*Hydrogen Quality Analysis: Production to Fuel Cell, ANL, Romesh Kumar*	3.19		X			The project complements other efforts to determine the effects of fuel contaminants on fuel cell components, and to set standards for fuel purity. The project is addressing a critical issue and has a reasonable approach.
AN-07	*Well to Wheel Analysis of Hydrogen Pathways with GREET Model, ANL, Michael Wang*	3.14		X			The model and analysis provides a clear understanding of well to pump, pump to wheels and well to wheels energy use, petroleum use and greenhouse gas emissions for many hydrogen pathways. The model assumptions should continue to be updated.
AN-08	*HyTrans Model, ORNL, David Greene*	3.47		X			The model provides the ability to investigate realistic strategies to enable the hydrogen rollout and explore the impact of policy on these strategies.
ANP-01	*Impact of Renewables on Hydrogen Transition Analysis, TIAX, Stephen Lasher*	3.43				X	The model is complete and will be used to analyze the most economic attractive renewable hydrogen production pathways. Additional work would involve the addition of coal gasification and natural gas reforming to the model technology portfolio.
ANP-02	*Hydrogen Analysis: H2A Update 2007, NREL, Todd Ramsden*	3.16		X			Excellent model for economic analysis of hydrogen production technologies. Provides for consistency and transparency of analysis. The model is being updated for scaling and updated technology information.
ANP-03	*System Dynamics: HyDIVE – Hydrogen Dynamic Infrastructure and Vehicle Evolution Model, NREL, Cory Welch*	2.78		X			The model is in the early phases of development. The project will help understand the number of refueling sites required for sustainable growth as a function of consumer choice and behavior. Representation of consumer actions and choice will be a significant determinant for the model.

Project No.	Project Title, Performing Organization, PI	Final Score	New	Continued	Discontinued	Project Completed	Summary Comment
ANP-05	*Analysis Repository, ATS, Melissa Lott*	3.21		X			Provides a single location for researchers to search for prior work/analysis associated with hydrogen related topics. The repository will dependent on the submission or retrieval of information.

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INTRODUCTION

This report is a summary of comments from the Peer Review Panel at the FY 2007 DOE Hydrogen Program Annual Merit Review, held on May 15-18, 2007, at the Gateway Crystal Marriott in Arlington, Virginia. The work evaluated in this document supports the Department of Energy (DOE), and the results of this merit review and peer evaluation are major inputs utilized by the DOE in making its funding decisions for following fiscal years.

The objectives of this meeting were to:

- Review and evaluate FY 2007 accomplishments and FY 2008 plans for DOE laboratory programs and industry/university cooperative agreements and R&D that supports development.
- Provide an opportunity for program participants (hydrogen production manufacturers, hydrogen storage manufacturers, fuel cell manufacturers, etc.) to shape the DOE sponsored R&D program so that the highest priority technical barriers are addressed. The meeting also serves to facilitate technology transfer.
- Foster interactions among the national laboratories, industry, and universities conducting the R&D.

The Peer Review process followed the guidelines of the Peer Review Guide developed by EERE. The Peer Review Panel members, listed in Table 1, attended the meeting and provided comments on the projects presented. These panel members are peer experts from a variety of hydrogen and fuel cell related backgrounds including national laboratories, hydrogen production manufacturers, hydrogen storage manufacturers, fuel cell manufacturers, universities, and other U.S. Government agencies. Each member was screened from a conflict of interest (COI) perspective per the Peer Review Guide. A complete list of the meeting participants is presented as Appendix A to this report.

Table 1: Peer Review Panel Members

No.	Name	Organization
1	Tarek Abdel-Baset	DCX
2	Jesse Adams	DOE
3	Kev Adjemian	Nissan Motor Company
4	Shabbir Ahmed	ANL
5	James Alkire	GFO
6	Michele Anderson	ONR
7	Mike Anderson	DOE-ID
8	Tim Armstrong	Oak Ridge National Laboratory
9	Radoslav Atanasoski	3M
10	Carol Bailey	SAIC
11	Balu Balachandran	Argonne National Laboratory
12	Bhaskar Balasubramanian	Chevron
13	Viktor Balema	Sigma-Aldrich
14	Olga Baturina	Naval Research Laboratory
15	Farshad Bavarian	Chevron
16	Bud Beebe	SMUD

17	Harold Beeson	NASA
18	Pierre Benard	Pierre U of Quebec
19	Thomas Benjamin	Argonne National Laboratory
20	Jeff Bentley	CellTech Power
21	Larry Blair	Consultant (retired from DOE)
22	Chris Bordeaux	Bordeaux International Energy Consulting, LLC
23	Silvia Boschetto	BP
24	Arun Bose	NETL
25	Lynnae Boyd	National Renewable Energy Laboratory
26	Robert Buxbaum	REB Research & Consulting
27	Mei Cai	GM
28	Jim Campbell	Air Liquide
29	Daniel Casey	ChevronTexaco
30	William Chernicoff	DOT - Volpe
31	Biswajit Choudhury	DuPont Fuel Cells
32	Larry Christner	LGC Consultant LLC
33	Deryn Chu	U. S. Army Research Laboratory
34	Bill Collins	UTC Power/Fuel Cells
35	Mario Conte	EC
36	Cecilia Cropley	Giner Electrochemical
37	Maria Curry-Nkansah	BP
38	Dennis Curtin	DuPont
39	Mark Debe	3M
40	Millie Dresselhaus	MIT
41	Daniel Driscoll	NETL
42	Glenn Eisman	RPI
43	Carolyn Elam	DOE
44	Mohammad Enayetullah	Protonex Technology Corporation
45	Gonzalo Escobedo	DuPont
46	Leslie Eudy	NREL
47	Dave Farese	Air Products
48	Christian Fau	Freudenberg-NOK General Partnership
49	Constantina Filiou	EC
50	James Fletcher	James
51	Scott Freeman	DaimlerChrysler Corporation
52	Robert Friedland	Proton Energy Systems Inc.
53	George Frudakis	George (Greece)
54	Alexi Gabrielov	Shell
55	Jennifer Gangi	Fuel Cells 2000
56	Craig Gittleman	GM
57	Bob Glass	Lawrence Livermore
58	Adam Gromis	CaFCP
59	Tom Gross	IF,LLC/LMI
60	Jill Gruber	DOE/GO

61	Nikunj Gupta	Shell
62	Steve Hamrock	3M
63	Jonathon Hardis	DOC/ NIST
64	Barbara Hennessey	National Highway and Traffic Safety Administration
65	Andy Herring	Colorado School of Mines
66	Steve Herring	INEL
67	Shinichi Hirano	Ford Motor Company
68	Kasuhiko Hirose	Toyota
69	Peter Hoffman	The Hydrogen & Fuel Cell Letter
70	Jamie Holladay	PNL
71	Doug Hooker	DOE
72	Ashraf Iman	Ashraf NRL
73	Brian James	Directed Technologies, Inc.
74	Puru Jena	VA Commonwealth University
75	Craig Jensen	U of Hawaii
76	Karl Jonitez	Karl LANL
77	Scott Jorgensen	GM
78	Karel Kapoun	Shell
79	Jim Kegerreis	ExxonMobil
80	John Kerr	Lawrence Berkeley National Laboratory
81	Tom Kimbis	DOE
82	John Kopasz	Argonne National Laboratory
83	Ted Krause	ANL
84	Benjamin Kroposki	National Renewable Energy Laboratory
85	Romesh Kumar	Argonne National Laboratory
86	Nobuhiro Kuriyama	Nobuhiro
87	Stephen Lasher	TIAX
88	Jay Laskin	Consultant
89	Lawrence Barton	University of Montana
90	Michelle Lewis	ANL
91	Ludwig Lipp	Fuel Cell Energy
92	Rob Lucchesi	ExxonMobil
93	Andy Lutz	Sandia National Laboratories
94	Maggie Mann	National Renewable Energy Laboratory
95	Robert Mantz	ARO
96	Victor Maroni	ANL
97	David Masten	GM
98	Thomas McNulty	GE Global Research
99	Shawna Mcqueen	Energetics
100	Paul Meier	ConocoPhillips
101	Jeremy Meyers	University of Texas at Austin
102	Eric Miller	University of Hawaii
103	James Miller	Argonne National Laboratory
104	George Mitchell	George

105	Rana Mohtadi	Toyota
106	Tom Moore	Consultant
107	Karren More	ORNL
108	Deborah Myers	Argonne National Laboratory
109	Yumiko Nakamura	AIST
110	Kevin Nguyen	Chevron
111	Frank Novachek	Xcel Energy
112	Greg Olsen	Consultant
113	Cathy Padro	Los Alamos National Laboratory
114	Pinakin Patel	FuelCell Energy, Inc.
115	Dilo Paul	NETL
116	Mike Perry	UTC Fuel Cells, LLC
117	John Peters	Montana State University
118	John Petrovic	Consultant
119	Bryan Pivovar	LANL
120	Walter Podolski	Argonne National Laboratory
121	C.G. Michael Quah	Concurrent Technologies Corporation
122	Martin Quintus	DaimlerChrysler AG
123	Kwan Quon	DOT
124	Venki Raman	Protium Energy
125	Vijay Ramani	Illinois Institute of Technology
126	Robert Remick	Colorado Fuel Cell Center
127	Vernon Roan	University of Florida
128	John Robbins	ExxonMobil
129	Jerry Rogers	General Motors Corporation
130	Neil Rossmeissl	DOE Office of Biomass Program
131	Dr. Samuels	Consultant
132	Gary Sandrock	Consultant
133	Steve Schlasner	ConocoPhillips
134	Jesse Schneider	DaimlerChrysler
135	John Shen	DOE
136	John Shewchun	Wayne State University
137	Neel Sirosh	Quantum Technologies Inc.
138	Dave Sjoding	Washington State University
139	Ed Skolnik	Energetics, Inc.
140	Sofronis Smith	Shell
141	Mike Sofronis	University of Illinois
142	Mike Steele	GM
143	Rhoads Stephenson	Safety Panel
144	Darlene Steward	NREL
145	Howard Stone	ARUP Energy
146	Ken Stroh	Los Alamos National Laboratory
147	Thanos Stubos	NCSR Demokritos
148	Andrea Sudik	Ford

149	Bill Summers	SRNL
150	Karen Swider Lyons	NRL
151	Hazem Tawfik	State University of New York & BNL
152	George Thomas	Consul.
153	Doanh Tran	Radiance Technologies
154	George Tsotridis	EC
155	John Turner	NREL
156	Nick Vanderborgh	Consultant
157	Keith Vanderveen	Sandia National Laboratories
158	Henry Voss	PolyFuel
159	Fred Wagner	Energetics
160	Jim Waldecker	Ford Motor Company
161	Sharlene Weatherwax	DOE
162	Steven Weiner	Pacific Northwest National Laboratory
163	Doug Wheeler	DJW Technology
164	Robert Wichert	USFCC
165	Barbara Wolfe	New West
166	Chris Wolverton	Northwestern Univ.
167	Chao (Tony) Wu	Southern Company
168	Jung Yi	Arkema Inc
169	Piotr Zelenay	LANL
170	Dick Ziegler	SENTECH, Inc.

SUMMARY OF PEER REVIEW PANEL'S CROSS-CUTTING COMMENTS AND RECOMMENDATIONS

The Peer Review Panel members provided a number of comments and recommendations that apply to the Annual Merit Review and peer review process, as well as overall management of the DOE Hydrogen Program. These comments are provided in Appendix C of this report. DOE will utilize these comments to improve both the program and future review meetings.

ANALYSIS METHODOLOGY

As shown above, **170** panel members participated in the merit review process. A total of **161** projects were reviewed at the meeting and a total of **977** evaluation forms were received from the Peer Review Panel (not every panel member reviewed every project). These panel members were asked to provide numeric scores (on a scale of 1 to 4, with 4 being the highest) for five aspects of the research on their Evaluation Form, a sample of which can be found as Appendix C.

The five criteria and weights were:

- Relevance to overall DOE objectives (20%);
- Approach to performing the research and development (20%);
- Technical accomplishments and progress toward achieving the project and DOE goals (35%);

- Technology transfer and collaborations with industry, universities, and other laboratories (10%); and
- Approach to and relevance of proposed future research (15%).

All the individual criterion scores from various reviewers were averaged together to obtain average scores for each of the five above-mentioned criterion for every project. These average scores were then weighted and combined to produce a final overall score for that project. In this manner, a project's final overall score can be compared to other projects. Following is the formula used to calculate the weighted average overall score:

*Final Score = Score1*0.20 + Score2*0.20 + Score3*0.35 + Score4*0.10 + Score5*0.15*

A few new projects were reviewed, where the third criterion (Technical Accomplishments) did not apply because of the project's recent startup. In this case, the other four criteria were scaled proportionally in the weighting calculation and the following formula was used:

> *Criterion 3/ Technical Accomplishments weighted at 35% not included; therefore, weighting value for remaining scores = (weight +35/65*weight)*
>
> *Final Score = Score1*(0.20+(35/65)*0.20) + Score2*(0.20+(35/65)*0.20) + Score4*(0.10+(35/65)*0.10) + Score5*(0.15+(35/65)*0.15)*
>
> *So, Final Score = Score1*0.31 + Score2*0.31 + Score4*0.15 + Score5*0.23*

A maximum final overall score of 4 signifies that the project satisfied the above mentioned five criteria to the fullest possible extent, while a minimum score of 1 implies that the project did not satisfactorily meet any of the requirements of the five criteria mentioned above.

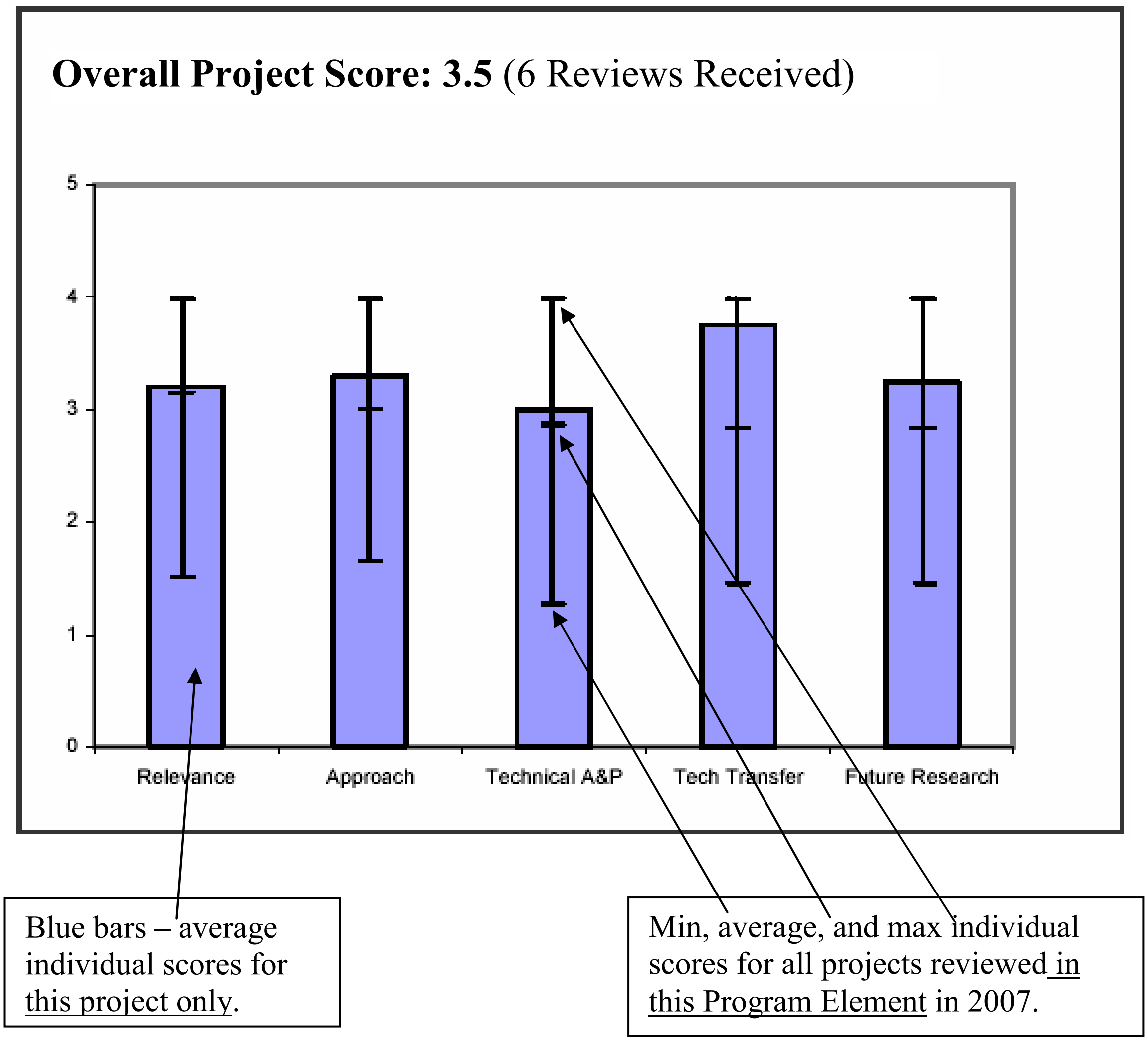
Reviewers were also asked to provide qualitative comments on the five research aspects, as well as the specific strengths and weaknesses of the project, and any recommendations for additions or deletions to the work scope.

These comments, along with the quantitative scores, were placed into a database for easy retrieval and analysis. These comments are summarized in the following sections of this report.

ORGANIZATION OF THE REPORT

This report is organized in seven sections, in an effort to group projects according to the program elements in which they fall in DOE Hydrogen Program planning. A brief description of the general type of research being performed in each category is presented at the beginning of each major report section.

The remaining pages of each section present the results of the analysis for each of the projects discussed at the merit review. A summary of the qualitative comments is provided, as well as graphs showing overall score and how the particular project compared with all other projects presented within each program category. An example of a graph is provided below:



The project comparisons illustrated in the report are criteria based. Each rectangular blue bar in the chart represents that project's score for that particular criterion of the project. The displayed score for each criterion of a project was obtained by averaging the individual reviewer scores for that particular criterion of the project.

This project's score for each particular criterion (each blue bar) was then compared with the maximum, minimum and average score for that same criterion of all the presented projects (across all sub sections of the Hydrogen program). The maximum, minimum and average scores for a criterion across all the presented projects is graphically displayed by the black line bars which overlay the blue rectangular bars.

For clarification purposes consider that only three projects were presented and reviewed. The hypothetical projects were scored by reviewers as displayed in the table below:

	Relevance	Approach	Technical A&P	Tech Transfer	Future Research
Project 1	4	2	1	4	3
Project 2	1	4	4	3	2
Project 3	2	3	2	1	4
Max	4	4	4	4	4
Min	1	2	1	1	2
Average	2.3	3.0	2.3	2.6	3.0

In this case, the chart for project 2 would contain a blue rectangular bar with a value of 1 (reflecting the score obtained by project 2 for the relevance criterion) and a black line bar with max, min and average values of 4, 1, and 2.3 respectively for the relevance criteria. Below is a sample calculation for the Project 1 weighted score.

*Final Score = 4*0.20 + 2*0.20 + 1*0.35 + 4*0.10 +3*0.15= 2.4*

2007
Hydrogen Production and Delivery
Summary of Annual Merit Review Hydrogen Production and Delivery Subprogram

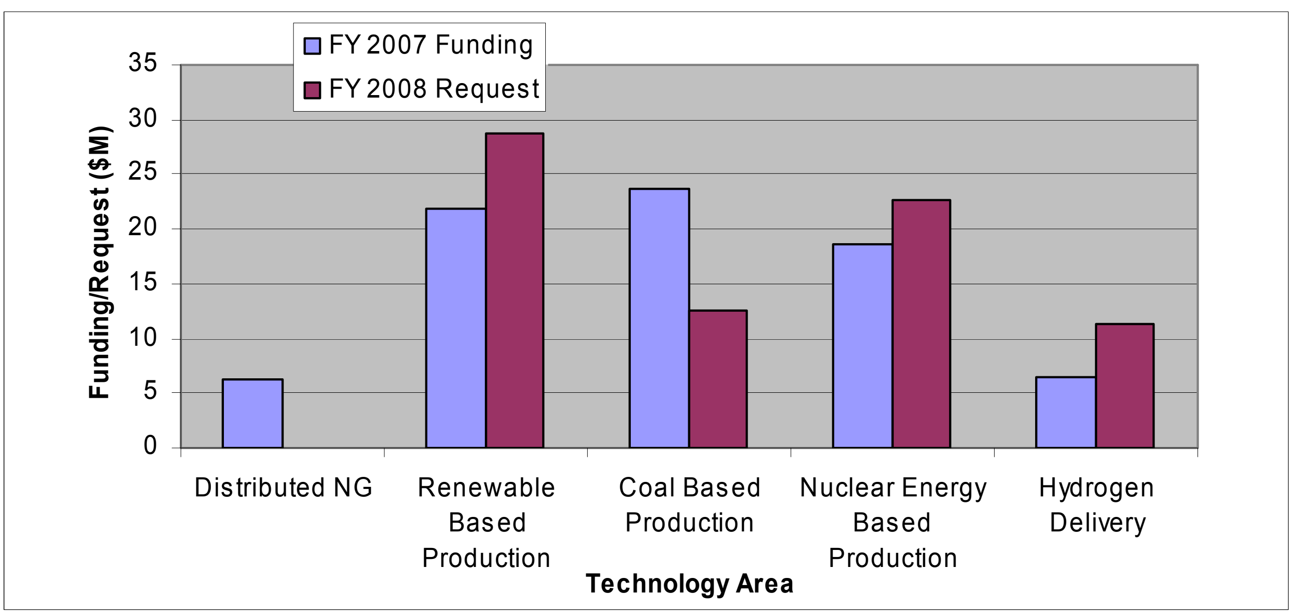
Summary of Reviewer Comments on Hydrogen Production and Delivery Subprogram:

This review session evaluated hydrogen production and delivery research from all DOE activities working on the President's Hydrogen Fuel Initiative, including: the Offices of Fossil Energy, Nuclear Energy, and Energy Efficiency and Renewable Energy. The production and delivery projects are generally considered to be well-aligned with the goals and objectives of the Hydrogen Program.

The production projects include diverse energy sources and technologies for hydrogen production including natural gas reforming, water electrolysis, bio-derived renewable liquids reforming, biomass gasification, solar-driven thermochemical cycles, nuclear-driven thermochemical cycles, photoelectrochemical direct water splitting, biological hydrogen production, and hydrogen production from coal. The projects were judged to have made considerable progress, despite a low level of funding in some areas. The major concerns identified in some projects by reviewers were: 1) collaboration roles with some industry partners and other research organizations need to be expanded and clarified; 2) some projects need to better define objectives to align with the program's technical targets; 3) more project test data and other technical information is needed to assess progress; and, 4) specific go/no-go decision points are needed on some projects.

The delivery projects reviewed included the next stage of development of the H2A Delivery analysis models, and several of the key hydrogen pipeline research efforts. The reviews were very complimentary of the advances made in the H2A models and recognized significant and very relevant progress in the pipeline research despite limited funding.

Hydrogen Production and Delivery Funding by Technology:



Majority of Reviewer Comments and Recommendations:

In general, the reviewer scores for the production and delivery projects were high to average, with scores of 3.6, 3.1 and 2.3 for the highest, average and lowest scores, respectively. The scores are indicative of the technical progress that has been made over the past year. Recommendations and major concerns are summarized below.

Distributed Natural Gas and Bio-Derived Liquids Reforming: Reviewers acknowledged that low cost forecourt (on-site) units are critical to meeting DOE Hydrogen Production objectives during the transition to use of hydrogen as a major energy carrier. In addition to reducing the footprint, it was stated that a remaining challenge for technology developers is to scale-up these highly efficient, small capacity reformers to achieve economies of scale that will enable the technology to reach the DOE target for distributed natural gas of $2-$3/gge by 2015. New technology being developed for distributed reforming from bio-derived liquids (e.g. ethanol, sugars) will build on distributed reforming from natural gas technology while helping solve outstanding issues with the on-site hydrogen production to reach the bio-derived liquids cost goal of $3.00/gge by 2017. While there were mixed reviews on the ability of the U.S. to provide sufficient bio-derived feedstocks for transportation energy needs, the majority were highly in favor of pursuing bio-derived liquids to hydrogen, praising technology efforts in distributed gas phase and aqueous phase reforming.

Electrolysis: Projects in electrolysis development received generally favorable reviews. The reviewers identified electrolysis using renewable energy as "one of the two most viable options for hydrogen production in the near term." Most of the projects were regarded as well-aligned with current program goals and objectives. Reviewers suggested increased collaboration with industrial partners and other DOE-funded projects. They stressed the need for decreasing the cost related to these systems, increasing system reliability and performance, validation of models, and continuing the work of integrating the electrolysis units with renewable energy sources such as wind power. Successful completion of these projects may yield multiple options for efficiently producing hydrogen from water and renewable energy at economically acceptable costs.

Biomass Gasification: Two projects in this area were reviewed; one researching the potential to integrate a hydrogen membrane in a biomass gasifier for process intensification and thus capital cost reduction; the other researching the potential of central plant, low temperature, single step, aqueous phase reforming of hydrolyzed biomass. Both projects received below average scores based on the fact that the projects are high risk compared to standard biomass gasification. These projects are just being initiated. If successful, either could substantially reduce the cost and complexity of central hydrogen production from biomass. They include early decision points for continuation of the work based on their risk level and progress.

Solar-Driven High Temperature Thermochemical: The large collaborative project reviewed in this area received very favorable comments. It was viewed as extremely relevant to the Program goals for renewable-based hydrogen production. There was significant research progress on the five down-selected thermochemical cycles. The reviewers urged the project to follow their plan to further down-select to 1-3 cycles in FY08 and encouraged additional work on materials research, and heliostat cost reduction.

Photoelectrochemical Hydrogen Production: The teaming approach in some of the projects in this area was specifically called out by the reviewers as effective and necessary to achieve the DOE targets. Several of the projects received high ratings from the reviewers. Nearly all the projects were viewed to be in-line with the program's long-term goals. The projects have achieved good scientific progress in materials research and have established effective collaborations. Reviewers suggested that increased research effort be devoted to materials durability and systems development, and that down-select decision points and criteria be established.

Biological Hydrogen Production: The projects in this area were rated very high and the general conclusion from the reviewers is that the researchers are moving toward the DOE goals in this long-term renewable hydrogen production area. Some reviewers suggested increased collaborations with industry to apply the exploratory results obtained from this project.

Separations: Reviewers commented, similar to prior year reviews, that there is a great need for investigators to test their hydrogen separation and purification membranes using realistic, mixed gas streams. The potential for membrane technology to reduce the on-site hydrogen production footprint (by eliminating PSA) and reduce capital costs were frequent comments. The ability of the research to be applicable to many hydrogen production technologies was viewed by many reviewers as advantageous. Some reviewers thought that technology advances in separations are not occurring quickly enough.

Hydrogen from Coal: The projects reviewed in this area received mostly favorable ratings from the reviewers. Reviewers observed that the projects were in alignment with the DOE Hydrogen Fuel Initiative and Hydrogen from Coal Program goals and objectives. The projects had achieved good technical progress and their overall research approach was determined to be solid. Reviewers observed that some projects needed to improve or highlight their technology transfer and partnership activities. Also, reviewers suggested that some projects need to focus on tests using more representative mixed gas streams to address issues regarding real-world applications

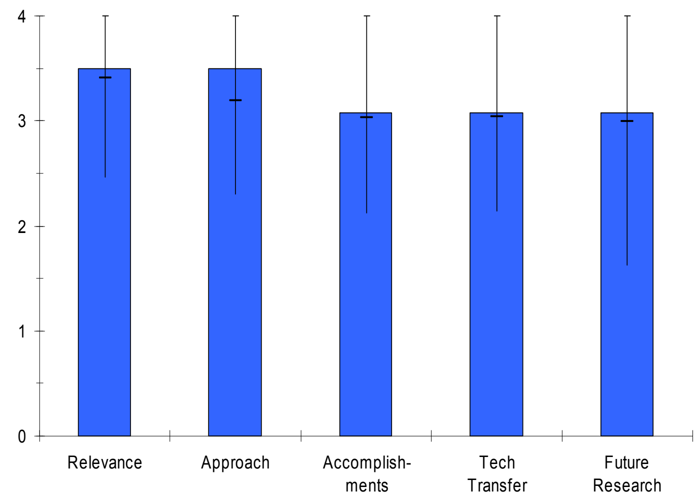
Hydrogen Production Using Nuclear Energy: In general, the projects reviewed in this area were scored favorably. Reviewers approved of the breadth of collaboration for some projects and the well-focused approach of other projects. The projects were judged to be well-aligned with the program's goals. Reviewers recommended that research be driven by materials and cost issues. Economic analyses and high-level assessments of licensing issues were also recommended as areas for future efforts.

Hydrogen Delivery: All but one of the projects reviewed in this area received above average ratings. The reviews recognized significant and very relevant progress in the pipeline research despite limited funding. They complimented the broad spectrum of collaboration across industry, national labs, and universities as well as a good mix of theory, modeling, and experimental work. There was enthusiasm for the fiber reinforced pipeline project as being a step out approach that could significantly lower capital cost and avoid the embrittlement concern of steel pipelines. Stronger and broader collaboration and a more inclusive set of testing were suggested for this particular project. Reviewers requested that one project improve alignment and reduce duplication with other current program activities.

Project # PD-01: Low Cost Hydrogen Production Platform
Tim Aaron; Praxair

Brief Summary of Project

Overall Project Score: 3.2 (7 Reviews Received)



Praxair is developing an integrated system for the turnkey production of hydrogen at 4.8 kg/h for transportation and industrial applications. The design is based on existing steam methane reforming technology and existing chemical processes/technologies to meet the design objectives. The baseline design, therefore, consists of a steam methane reformer, pressure swing adsorber system for hydrogen purification, natural gas compression, steam generation and all components and heat exchangers required for the production of hydrogen. The focus of the project emphasizes packaging, system integration and an overall step change in the cost of capital required for the production of hydrogen on site. One objective of the project is to approach the DOE hydrogen cost goal of $1.50-$2.00/kg (production only).

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

- Low cost forecourt units are critical to meeting DOE objectives.
- Strongly supports near term goal for natural gas distributed reforming; Phase 3 necessary for evaluation of technology in an overall, integrated system.
- Directly addresses production program goal of reducing cost of distributed natural gas reforming via capital cost reduction.
- Program clearly addresses the goals of the DOE H_2 Program.
- Design for manufacturing has been implemented well to reduce capital cost.
- Good design for turndown to support market demand.
- Good concept with small footprint for distributed applications.
- Addresses several technical barriers identified by DOE in the areas of hydrogen production and technical validation.
- Supports distributed production of hydrogen for transportation application.

Question 2: Approach to performing the research and development

This project was rated **3.5** on its approach.

- Approach is well designed.
- Drawn out schedule may cause inefficiencies.
- Use of BDI and manufacturing contractor rounds out team.
- Work on codes and standards ISO committee augments knowledge.
- Good approach; good effort reducing part count and manufacturing cost; questionable scale-up to 1500 kg/day.
- Solid approach designed for success.
- Sound engineering, catalysis, and packaging to produce a product that should perform.
- Capacity is small compared to new DOE production program target...but they are building what they were contracted to build...and demonstrated in the presentation that there might be an important niche for 120 kg/day hydrogen generators for smaller stations in the early stages of infrastructure rollout.

- Approach is well thought out and comprehensively addresses safety, construction and operation.
- Good use of off-the-shelf technology (i.e., commercially available burner instead of custom design). Integrating off the shelf technology saves time, money and increases reliability.
- In a growing market, makes sense to have small unit and add units as demand increases.
- Unclear approach for 700 bar compression needed more information.
- Toxic emissions from reformer due to lower residence time were not discussed.
- Unclear who will commercialize, provide service, and whether this is a licensing application.
- The process is quite standard and would serve well as a demonstration project.
- Focus on manufacturability is a good strategy effectively addressing the manufacturing barrier.
- Tried to address the reformer capital costs. The projected cost estimate of $2.75/Kg of H_2 is on the higher side of DOE cost goals.
- Plan to address codes & standards but not much is done.

<u>Question 3: Technical accomplishments and progress toward project and DOE goals</u>

This project was rated **3.1** based on accomplishments.

- Using commercial catalyst.
- Not completely proven, but if catalyst is shown to be good for full 7.5 yr design life, then it would be a significant design feature.
- More data (beyond costs) compared to goals would be helpful; Need demonstration phase for insight into performance parameters (reliability, durability, etc.).
- Work appears to be on track. Their cost models indicate they might meet DOE targets even with systems that have this low capacity.
- Skid appears to be well designed; easy access to components for ease of maintenance.
- Significant accomplishments achieved including approaching H_2 cost, durability.
- Good accomplishment on catalyst selection. Unclear about the long term reliability of the PSA unit at the 50 percent turndown rate. More accelerated testing should be done to verify performance and cost values.
- Reformer and shift catalyst testing data has been shown but it is not very revealing of progress. H_2 yield data, durability, space velocity, durability, etc., would be more meaningful.
- Cost of hydrogen has been estimated but does not include compression costs.
- Completed techno-economic study, proof-of-concept component testing and most of lab-scale testing.
- Full-scale test apparatus constructed. Off-the shelf components used wherever possible & highly integrated system (addresses the fuel processor capital costs barrier). Risk analysis completed (Control and Safety barrier addressed).

<u>Question 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **3.1** for technology transfer and collaboration.

- Minimal collaborations; much focus on Praxair.
- Good coordination of work with component vendors and suppliers. Collaborated with Boothroyd Dewhurst and Diversified Manufacturing to develop component selection and manufacturing strategies to get parts count and manufacturing costs down.
- Good to see collaboration with two experienced companies on design and construction, otherwise appears to be light on collaboration and technology transfer.
- Coordination, but insufficient info on how it's used to deal with cost or performance problems.
- They are working with commercial catalyst vendors and manufacturing.
- They have a manufacturer on the team.
- Boothroyd Dewhurst is in charge of system optimization. Diversified Manufacturing is in charge of manufacturing the skid and prototype.
- Praxair has good track record in commercializing technologies. Praxair is the only U.S. H_2 supplier in all sizes (cylinders to liquid to pipelines).
- Praxair has smallest industrial SMR-based product line. They have designed and built over 300 PSA H_2 units.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.1** for proposed future work.

- A demonstration phase would be useful; especially with start-up/shutdowns, transients, etc; daily usage profile important as system appears designed for steady-state performance; no discussion of role of storage in Phase 3.
- Project is well planned; future proposed work will add great value to achieving future commercialization.
- Unclear how reformer will perform with normal variance of natural gas composition, especially if higher levels of carbon dioxide.
- Presumably the team has enough experience in hydrogen production using this standard process. Unclear why the team would spend resources on natural gas compression and high temperature materials.
- This reviewer was confused regarding the plan for testing of components/proof of design. At first this reviewer was led to believe that the proof-of-concept component testing was completed during Phase I of this project. Unclear why this would be done again.
- This team plans to perform comparative analysis with supply alternative (considers contingencies).

Strengths and weaknesses

Strengths
- Project is right on target for what needs to be done for low cost forecourt NG reformer systems.
- DFMA methodology is good to employ.
- Good effort reducing parts and designing for manufacturability; good cost reduction.
- Good use of existing technology to address near term transition to H_2.
- Strong team with strong technical performers
- Used past failures on small reformer technologies to develop an impressive concept.
- Good management visibility.
- This is a demo of a pretty standard process that is most likely to be commercialized in the near-term, and so it is an important project for data generation.
- Praxair has experience in smallest industrial SMR-based product line. They have considerable experience with PSA H_2 units.

Weaknesses
- Too little detail is in presentation: Unclear about efficiency, life (cycle) testing, and the capital cost not just the bottom line cost of hydrogen.
- Questionable scale-up to 1500 kg/day design; proposed solution of multiple units could result in reliability issues (undoes effort to reduce part count).
- Commercialization plan and market study needed.
- No real data. Catalyst performance data could be more elaborate. There should be more information contributed to the public domain.
- Co-content in H_2 was not addressed properly. The purity of hydrogen may not be suitable for PEM application.
- Thermal cycling will be a problem for this small reformer.

Specific recommendations and additions or deletions to the work scope

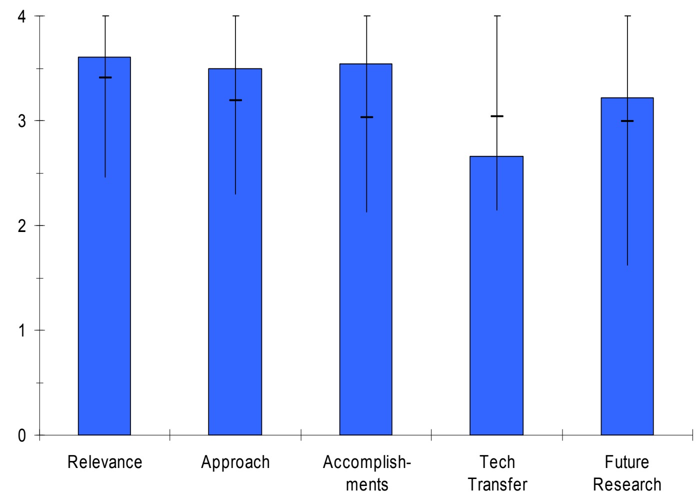
- As part of a demo, test under daily usage profile similar to H2A assumption.
- Adding the demonstration of 700 bar hydrogen is a good addition of project scope in that it pushes the envelope of standard practice and will generate data on cost of the product and the overall process efficiency at those conditions.
- Need to firmly establish ease of maintenance and operation to be accepted by industry.
- Based on other reformer projects more accelerated performance testing to validate small scale reformer/PSA unit cost and reliability.
- Need to document the contaminants, their level, and the impact on cost of hydrogen.
- Address CO_2 issue.
- Longer-term data are needed.
- Can this team increase the purity of the H_2 from their unit (CO less than ppm level)?

Project # PD-02: Low-Cost Hydrogen Distributed Production Systems
Frank Lomax; H2Gen Inno. Inc.

Brief Summary of Project

H2Gen Innovations is conducting the development, fabrication and testing of an advanced steam methane reformer and pressure swing adsorption (PSA) system that will produce ~10,000 scfh (565 kg/day) of 99.999% pure hydrogen at over 200 psig, to meet the DOE 2010 interim cost target of $2.50/kg. A catalyst suite suitable for use with fuel grade ethanol to facilitate renewable hydrogen production is also being developed.

Overall Project Score: 3.4 (5 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.6** for its relevance to DOE objectives.

- Strongly supports natural gas distributed reforming goals; more feedback concerning performance versus goals necessary.
- Project clearly meets the DOE Hydrogen Program targets.
- Good concept to achieve high reliability and cost.
- Meets the need for renewable hydrogen production from ethanol.
- Management understands and appreciates the requirement to achieve the DOE cost targets and is on track to meet them.
- Can be used for distributed and stationary applications.
- A demo of the natural gas to hydrogen process is appropriate for the near-term.
- H2Gen is not a catalyst company. Not clear about their novel concept for ethanol catalysis.
- This project addresses barriers such as fuel processor capital cost, manufacturing, O&M, feedstock issues, and control and safety in the Multi-Year RD&D plan.

Question 2: Approach to performing the research and development

This project was rated **3.5** on its approach.

- Development of natural gas reforming is well designed; addition of ethanol research, primarily the conversion from ethanol to methane is questionable.
- Well conceived, staged approach; sufficient testing of individual components.
- Good design and operations estimates.
- Could not tell if there were independent analyses on cost.
- Ethanol R&D looks promising.
- The process approach is good and makes sense for a refueling center.
- Fuel process capital cost, manufacturing costs, O&M, feedstock issues, and control and safety barriers are addressed in this project.
- This team has perfect approach.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.5** based on accomplishments.

- Strong accomplishment towards achieving cost targets; more performance parameters versus goals required.
- Impressive accomplishment to complete 565 kg/hr platform.
- Good progress and cost reduction.
- Materials of construction - limited data on reliability.
- Compression related work not clear to achieve cost.
- Good performance of reformer as demonstrated by data.
- New PSA designed to increase capacity.
- Not much data to evaluate technical progress.
- Unclear on Slide 8, where a plot is shown without any y-axis, what is being measured.
- Cost analysis is promising.
- Ability to convert ethanol is not very meaningful. Unclear how much H_2 and what else is produced.
- This team has made excellent progress toward meeting their overall objectives.
- Based on test experience at 113 Kg/day scale, they have redesigned reactor and flowsheet for 565 Kg/day platform. This system has low pressure drop burner, compact and low stress steam generator and linear combustion air supply system.
- To reduce risk and cost this team has tested the burner, steam generator, and air supply system at full 565 Kg/day scale.
- Designed skid to industry standards.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.7** for technology transfer and collaboration.

- Minimal collaboration; nearly all technology in-house.
- Good coordination, but commercialization and service support were unclear.
- Team roles unclear once R&D goals are achieved.
- Unclear how IP shared in the next generation technology.
- Partners have been identified for future site location.
- Sud-Chemie is a good partner, possibly in catalysis research.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.2** for proposed future work.

- Scale-up of approximately 115 kg/day unit to 565 kg/day will provide useful information and potential path to 1500 kg/day.
- Need to (eventually) have clear reasons/objectives for building the 2nd generation plant; should be based on a clear need with significant performance benefits.
- Good focus on research goals, accelerated reliability studies should be considered to validate longer term cost projections.
- The 565 Kg hydrogen generator will be tested at field site as well as building and testing a second 565 Kg hydrogen generator at a second field site.
- Based on test data, they will identify areas for improvement – excellent plan.
- In addition to the primary objective of reforming natural gas, H2Gen has secondary objective of using ethanol as a feedstock. They have plans to demonstrate the durability of ethanol reforming catalyst.
- They will make go/no-go decision based on durability tests.

Strengths and weaknesses

Strengths
- Simple design, skid mount approach useful.
- Good team with strong technical expertise. Past experiences have influenced current project and management oversight is good.

- Natural gas to hydrogen plant demonstration is promising with respect to cost targets.
- Very good project planning and execution.

Weaknesses

- Requires integration into overall production, compression, and storage system to determine transients, turndown, etc.
- Scale up from 113 to 567 was not clearly defined as to risk both on a market penetration basis and reliability of performance. Unclear whether the availability of components is within their current analysis or if a new evaluation will be undertaken since there is limited performance data available.
- Catalyst development strategy does not fit with this project.
- Unclear if it is necessary to pre-reform ethanol.
- No safety and code analysis for the installation of the hydrogen generator at the field site.

Specific recommendations and additions or deletions to the work scope

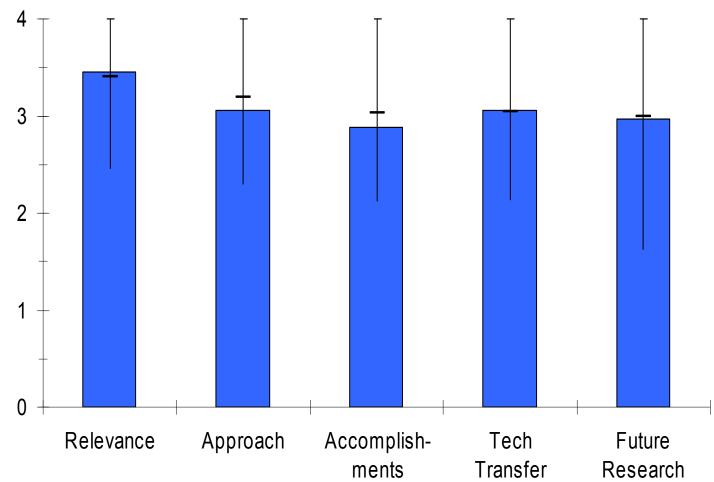
- Continue to complete this project to benchmark progress to goals.
- Add task to track hydrogen quality and its impact on cost of hydrogen.
- Maybe they should focus on their primary objective which is the development of hydrogen generator for distributed production of hydrogen using natural gas as feedstock. Would like to see more of these hydrogen generators built instead of redirecting their effort on reforming ethanol.
- It is a good idea for DOE to fund H2Gen for ethanol reforming.

Project # PD-03: Integrated Hydrogen Production, Purification & Compression System
Satish Tamhankar; Linde

Brief Summary of Project

The goal of this project is to demonstrate a low-cost option for producing fuel cell quality hydrogen that can be adopted to meet the ultimate DOE cost and efficiency targets for distributed production of hydrogen. The project team will develop a fuel processor system that directly produces high-pressure, high-purity hydrogen from a single integrated unit. This will be accomplished by combining a membrane reformer developed by Membrane Reactor Technology and a metal hydride compression system developed by HERA USA in a single package. In 2006/2007 the objective was to build and experimentally test a proof-of-concept integrated reformer/metal hydride compressor system.

Overall Project Score: 3.1 (6 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

- Success in the project would have significant positive effect on hydrogen cost.
- Novel approach; potential to simplify overall system; probable high risk.
- Project clearly meets the objectives of the DOE Hydrogen Program.
- Good to simplify process and reduce components.
- Capital cost reduction.
- Good solid state design compressor.
- Existing industry is important to DOE success if they will commercialize and service units.
- Addresses DOE identified technical barrier.
- Project is appropriate for near-term refueling centers.
- This project's objective is to develop a fuel processor system that directly produces high pressure, high-purity hydrogen from a single integrated unit and therefore has good relevance to overall DOE objectives.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- Not clear how waste heat of compressor is used to aid reformer.
- Minimal test data presented; only benchtop component testing to date.
- Novel approach to addressing the problem of H_2 production from CH_4.
- Well conceived plan to build an initial proof-of-concept prototype and then an advanced prototype based on learnings.
- A novel approach is only beneficial if there are clear advantages over conventional technology; need a head-to-head comparison with conventional technology.
- Good plan for hazmat and resulting improvement to safety.
- Higher costs due to design modification for hydride compressor.
- 10 week setback was unplanned? How did management deal with impact instead of sitting on their hands?
- Good progress on technical barriers.
- How much has been completed on market penetration studies?

- Novel approach offers opportunity for new technologies.
- H_2 removal membranes have not been demonstrated with high flux.
- H_2 permeating membranes yield low pressure hydrogen.
- Reforming at pressure with H_2 permeation can lead to carbon formation in the reformer unless operated at high steam to carbon ratio. The latter penalizes system efficiency.
- Metal hydride compressor is novel.
- Addresses fuel processor capital costs, O&M, and reliability and costs of hydrogen compression barriers by building an integrated fluidized bed reformer and metal hydride compressor system. Process intensification will bring the cost down to DOE target levels.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.9** based on accomplishments.

- Substantial achievement in completing mechanical design and fabricating system.
- Longevity/membrane attrition testing mentioned during the question period but details not available.
- Minimal accomplishments to date (based on presentation); lifetime questionable; path towards high pressure output (10,000 psi) unknown; more information of performance versus goals necessary, especially efficiency.
- Significant accomplishment to construct the proof-of-concept prototype.
- MHC performance needs to be directly compared to conventional compression costs (operating and capital cost).
- Benefits of fluid bed reformer need to be clearly compared to conventional reforming technology.
- Behind schedule at go/no go decision, and management planning for schedule recovery is unclear.
- Revised safety plan was good.
- Only one data plot, and without the unit for flux.
- The projected efficiency and other performance parameters should be listed. Q&A revealed efficiencies in the "mid-70s" at a steam to carbon ratio of 3, and it is unclear how this is defined. Unclear what is included in the efficiency calculations.
- Unclear if energy losses are associated with the hydride compression technology.
- Pros and cons of reformer skid assembly addressed.
- Auto-thermal fluidized bed membrane reformer assembly has been fabricated and installed.
- Pd-membrane has been tested at operating temperature and pressures but not using reformer product streams.
- Completed appropriate safety reviews.
- Review comments from last year's review were addressed.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- Good collaboration between partners; good use of capabilities.
- Appears to have close collaboration, however seemingly limited to industry.
- Unclear about the cause of delays and how it was communicated to team members.
- Unclear how catalyst life is (still a problem) is being addressed.
- Unclear who is responsible for market plans and commercialization.
- The presentation time is better utilized with one speaker with others participating in Q&A.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- Minimal testing of integrated system; integration of components could be challenging.
- Future work is properly dependent on success with POC prototype.
- Project should proceed only if clear benefits for novel approach are established and communicated.
- Accelerated reliability should be considered to determine impact on cost.

- Unclear what technology life cycle costs are.
- The project end date is June 2008. By the end of May 2007 this team plans to complete site installation of reformer.
- MHC will be commissioned for one month of integrated testing. Unclear if one month of testing is sufficient to gather all relevant data needed to move forward.
- It would be helpful to provide future plans after the completion of this project.

Strengths and weaknesses

Strengths
- >200 compression ratio, release at 1500psi is very good.
- Able to operate at lower temperature due to hydrogen removal.
- No coke formation.
- Good technical team, teaming arrangement and strong management group.
- The combination of membrane and hydride compression is novel.
- The cartridge system for membrane is nice. Unclear if these can be hot swapped.
- Lower capital cost possible compared to conventional fuel processors by reducing component count and sub-system complexity.

Weaknesses
- Need to elaborate on the benefit and cost (energy, efficiency).
- Not clear how Pd membrane separator will ever be cost effective.
- Contaminants getting through the membrane will contaminate the hydride reactor. Unclear if there is an option for a guard bed.
- Should have shown membrane long term tests results.
- Where is capital cost estimate? What about substrate cost?
- Minimal time for integration and testing.
- Higher cost of operation.
- System efficiency appears lower than conventional.
- Not much data has been shown.
- How much sulfur can the membrane tolerate?
- No reason given for the delay in getting the MHC skid ready.
- Unclear what the "Advanced Prototype" is. And what will happen to this project after this phase of the project ends in June 2008.
- Membrane life and catalyst durability are of significant concern.

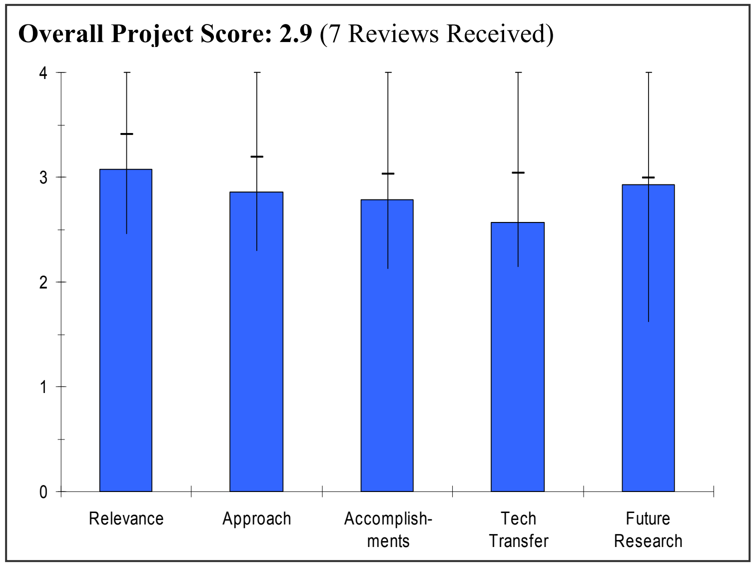
Specific recommendations and additions or deletions to the work scope

- More testing of integrated system needed.
- Independent risk assessment of concept needed.
- Flux data should not be proprietary. This is a performance parameter that has a target defined by DOE, just like parameters such as efficiency.
- Reviewers change or may not remember details from the previous year. Some information such as expected performance, if presented in past years, is worth repeating.
- Add the ability to track the effect of process conditions on contaminant levels, and ultimately on the cost of hydrogen.
- Test the membrane and catalyst under "real-world" application conditions before integrating the membrane reactor with the MHC.
- Provide commercialization plan for this system.

Project # PD-04: Bio-Derived Liquids Reforming
Yong Wang; PNNL

Brief Summary of Project

The objective of this project is to assist DOE in evaluating and developing alternatives to gasification and pyrolysis of biomass for hydrogen production that can meet the DOE 2017 cost target of <$3.00/gge. The objectives for FY 2007 were to develop stable and selective catalysts for vapor phase reforming of ethanol to produce hydrogen and to understand the reactivity and selectivity of aqueous phase reforming intermediates to enhance hydrogen productivity. An isothermal aqueous phase reforming reactor has been developed to screen catalysts and understand reaction mechanisms for improved hydrogen productivity.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.1** for its relevance to DOE objectives.

- Early evaluation of catalyst performance for reforming of bio-derived fuels, important topic as research moves beyond natural gas fuel processing.
- Project directly addresses Program goal of hydrogen production from renewable biomass resource.
- Potential long term solution to distributed reforming system with very low well to wheel CO_2 emissions
- Meets the DOE Hydrogen Program goal of cost effective H_2 production from bio-liquids.
- Presentation went into excessive detail on liquid phase reforming; needed to be balanced with how this technology has the potential to meet DOE H_2 production targets.
- Project is critical to the realization of renewable sources for hydrogen at the DOE targeted production cost of $3.00/gge by 2017. However, looks complimentary or redundant to Virent efforts in catalyst optimization.
- Critical to evaluate bioliquids as a feedstock for hydrogen.
- Capital cost reduction is critical for any hydrogen system.
- It is not clear whether any of the biofuels to hydrogen pathways shown make sense from a cost or efficiency perspective (i.e., there are probably more efficient ways to use biomass/biofuels).
- Ethanol is not competitive with gasoline without needing significant subsidies.

Question 2: Approach to performing the research and development

This project was rated **2.9** on its approach.

- Gas phase system approach not clearly presented.
- APR approach is well defined and effective.
- Need better definition of goals; minimal information provided on reactor rig and test plan; clear direction not presented.
- Very strong science focus on understanding catalytic fundamentals in this relatively unexplored system, including assessment of heat/mass transfer, identification of chemical intermediates, and exploration of potential reaction network.
- Concentrating on vapor phase ethanol because it is a current infrastructure fuel; will need to be extended to other bioliquids.
- Makes sense to explore liquid phase reforming; has obvious potential cost advantages.

- Good summary on current state of catalyst development. It appears that both PNNL and Virent are working on improving hydrogen selectivity for the Virent catalyst. So far the Virent catalyst has the best performance.
- Good that PNNL (and Virent) are working on processing low cost sugars with their catalyst.
- Fundamental mechanistic studies are well planned.
- Plan was not well explained.
- Unclear how team members were selected and how is each performing.
- Management review was unclear.
- Project doesn't seem focused on any of the barriers except identifying better catalysts.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.8** based on accomplishments.

- Hard to assess progress since specific goals not well defined.
- Very early in evaluation process; catalyst showed comparable performance.
- Tremendous amount of work done including:
    - Development of isothermal reactor (need this for mechanistic and kinetic studies).
    - Identification of stable and selective catalysts.
    - Complete product identification.
    - Mechanistic studies and influence of added KOH on overall reaction network.
- Demonstration of liquid phase reforming is a significant accomplishment; however, seems that the reactor productivity is very low (1-4 g feed/g catalyst/hr). Exploratory research notwithstanding, it is unclear how these levels of production will be commercially viable.
- Liquid phase reforming needs to be put in perspective with what catalyst advances would be required to meet DOE H_2 cost targets.
- Appears that a significant amount of work has been done to understand liquid phase reforming and many leads were generated on how this technology can be improved.
- The findings that microchannels, higher space velocity, and pH control can improve hydrogen conversion for the RePt catalyst may be important information to industry.
- Unclear if the project was reviewed for safety.
- No progress has been made on cost or efficiency – which were identified as barriers addressed.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.6** for technology transfer and collaboration.

- Minimal to date, but attempting to bring in more partners.
- Claim collaboration with Virent, but wasn't clear from the presentation what that partnership involves.
- Same goes for claimed collaboration with Ohio State research group...not clear what the nature of the collaboration is.
- Good collaboration with ANL and Ohio State.
- This seems to be limited in terms of collaborative influence. They are still not sure of likelihood that oil and ethanol producers will find value in project.
- Catalyst issues still a problem.
- Unclear whose responsible for carbon monoxide and other emissions.
- While numerous presentations appear to have been given, it is not clear if significant interactions occurred.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.9** for proposed future work.

- Future work for 2008 lacks specific targets for each planned task.
- Typical catalyst testing of selectivity, stability, etc.; planning to evaluate impurities. Evaluation of potential system performance would be helpful.

- Plans include minimizing acid formation, developing kinetic models, improving catalyst activity, selectivity, stability and developing process economics.
- The first two represent valuable and sensible science development at a national lab. Skeptical about the latter two activities and if these reflect appropriate activities for a national lab, when industrial labs are now pursuing these same targets. If PNNL is successful in developing promising new catalysts, it is unclear who will develop them.
- Mentioned performing a comparison with DOE cost targets; needs to be done sooner rather than later.
- Because the benefits of liquid phase reforming are great, work should continue to advance this technology.
- Future research to focus on larger reactor is sound if catalyst life and selectivity can be improved.
- Needs more clarification on go/no go decisions for different approaches.
- There doesn't appear to be appropriate off-ramps if the project results are not promising.

Strengths and weaknesses

Strengths
- Initial effort to evaluate vapor versus aqueous reforming of bio-derived fuels.
- Building basis of strong catalyst fundamentals in this new catalysis area.
- PNNL has good experience with small scale reformer R&D.

Weaknesses
- Very academic presentation: lots of information without much analysis of its significance. Made it hard to deduce true worth of work.
- Require better definition of goals and projected performance.
- Appears to be on a path to try and optimize catalyst life, activity, and selectivity, which would put it in competition with research going on in industry.
- Not sure of the differentiating benefit of this project here unless the Virent catalyst is just used as a baseline comparator.
- Market evaluation.
- Risk assessment.
- Commercialization.
- Very difficult to follow and understand the presentation.

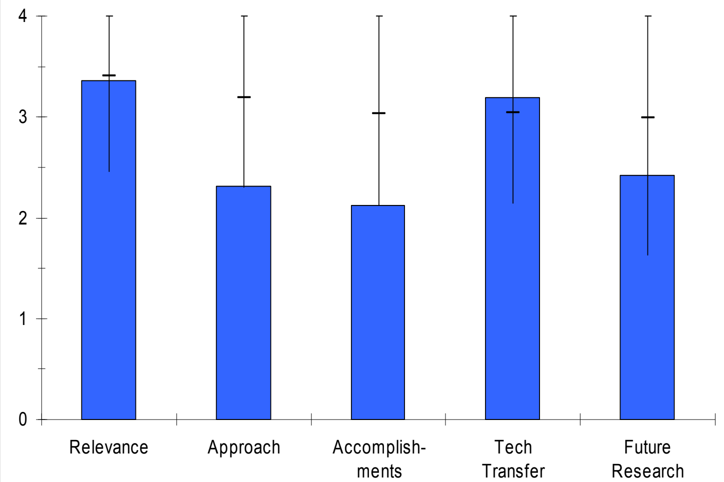
Specific recommendations and additions or deletions to the work scope

- No comment as no clear path forward presented.
- The project needs to perform preliminary cost and "well to farm to wheel" efficiency assessments to compare to other options (like using ethanol efficiently in an ICE) in order to establish performance targets for go/no-go decision points.

Project # PD-05: Biomass Gasification
Michael Roberts; GTI

Brief Summary of Project

Overall Project Score: 2.6 (7 Reviews Received)



The objectives of this project are to 1) reduce the cost of hydrogen produced from biomass gasification to \$1.60/kg H_2 (at the plant gate); 2) develop an efficient membrane reactor that combines biomass gasification, reforming, shift reaction and H_2 separation in one step; 3) develop hydrogen-selective membrane materials compatible with the biomass gasification conditions; and 4) demonstrate the feasibility of the concept in a bench scale biomass gasifier. Thermodynamic analysis indicates that there is potential for over 40% improvement in H_2 production efficiency over the current gasification technologies. The scope of the project includes membrane material development (ceramic, metallic, and composite materials), gasification membrane reactor process development and economic analysis, and bench-scale biomass gasifier design and construction.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.4** for its relevance to DOE objectives.

- Co-production of H_2 with renewable energy facilities economically viable on their own is an important initiating pathway for commercial H_2 as an energy carrier. Fluidized Bed (FB) gasification of biomass is one such opportunity, but impurities, variability of feedstock, and ash present significant challenges. This project begins to address several problems.
- A single step reformation-shift-separation method has shown advantages in other feedstreams (syngas), and is a reasonable goal for biomass as well.
- Addresses Program barriers: H_2 Production from biomass and related challenges in increased efficiency, impurity tolerance, and H_2 membrane targets of improved selectivity, flux at low temperature and impurity tolerance.
- Has not demonstrated that membrane approach has advantages over conventional biomass gasification/reforming (multiple reactors or combined).
- Biomass will be an important contributor to the hydrogen future.
- Relevant since it tries to use low cost biomass as fuel.
- Hydrogen from biomass is a renewable pathway. Solids handling and feed diversity are challenges for this feedstock.
- The project aligns well with the MYPP for a central production facility.
- The project offers the opportunity for CO_2 capture from biomass — more than a zero greenhouse gas emission approach, rather, a negative GHG emissions approach.
- The technology proposed has a high risk, high return nature appropriate for DOE support.
- Project objective is to reduce the cost of hydrogen from biomass to \$1.60/Kg H_2 (without delivery) and therefore there is relevant to overall DOE objectives. The project objective will be met by developing an efficient membrane reactor that combines biomass gasification, reforming, shift reaction and H_2 separation in one step.

Question 2: Approach to performing the research and development

This project was rated **2.3** on its approach.

- The initial spectrum of four types of membrane transfer types is the right place to start this project.
- The apparent initial plans to first evaluate all membrane types and then to begin in-reactor evaluation is not as expeditious as having at least some in-reactor experience earlier. Critical additional challenges to membrane media working in biogas will likely reveal additional limitations on membrane design not anticipated when designing to theory or synthetic biogas.
- Down-select criteria and process were not apparent.
- As this reviewer heard the approach: the target is a biomass gasifier with in-situ removal of hydrogen via a hydrogen permeable membrane. The goal is to enable gasification at lower temperature which in theory could improve efficiency.
- Not discussed in the talk is the fact that biomass gasifiers make much more oil and tar when operated at low temperatures. These are materials that we expect would at the very least form liquid films on the membrane modules and at least inhibit hydrogen transport (by adding a liquid film transport requirement) and possibly foul the membrane by poisoning.
- Fundamental knowledge of chemistry at these temperatures should lead to the EXPECTATION that the membranes will be fouled by reaction with one or more of the following: Cl, S, N, and liquid alkali oxides/hydroxides. The project tasks should be modified to set a much higher priority on demonstrating membrane stability to all these impurities before they are scaled up to the full scale expected for integration in the gasifier.
- Membrane won't be 100% selective for H_2. Plans for polishing? Small PSA?
- Alkali condensation on the membrane at these temperatures is a very serious concern. What is the temperature at the membrane?
- Reforming of methane is favored at high temp, while WGS is favored at low temp? Project should include thermodynamic simulations to determine equilibrium; pulling off the H_2 will solve part of this problem, but temperature is still important.
- What about dust clogging the membrane? Might be better to have some cyclone separation before the membrane.
- Many membrane scientists on team. Good combination of scientists but no party that knows how to make or commercialize membranes.
- The project uses a hydrogen membrane to remove the hydrogen. This may aggravate the prospects of coking the reformer if not accompanied with a high steam to carbon ratio. The latter penalizes system efficiency.
- The hydrogen yield is at a low pressure.
- GTI is experienced in biomass processing. That leaves the project revolving around the membrane. Membrane studies should be the highest priority and should be followed with a go/no-go after Task 2.
- Is oxygen feasible, cost wise?
- Substantial efforts by others have gone into applying H_2 membranes to cleaner environments than biomass gasification (e.g., natural gas SMR, WGS), yet none has achieved significant commercial success. Applying H_2 membrane technology to an environment as complex and dirty as a biomass gasifier presents a substantially greater challenge. Early, extended exposure of membranes to real (not simulated) gasifier conditions is important to reduce risk. The investigator does not plan to perform such tests until relatively late in the project.
- Presentation did not differentiate how this project's approach differs from previous projects' approaches (e.g., membrane SMR technologies) that were not successful.
- Chances of developing a membrane that can perform inside the biomass gasifier are low.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.1** based on accomplishments.

- Since the project has just received its first funding, progress beyond getting funding is not expected.
- Not really applicable...project just got started.
- Need a better PFD. Cannot possibly be working off the one presented. Not detailed enough and contains an error (only one gas stream out).

- What pressure does the H_2 come out at? Will need compression. Team should do a better job of understanding the entire system.
- Why hasn't a detailed cost analysis been done?
- What is the source of the cost data presented?
- Work done on breaking down H_2 cost from biomass not clearly based on own work. No references. Is this their work?
- Claimed 40% efficiency improvement over conventional biomass reforming. What is the anticipated efficiency?
- No data yet. Funding delays.
- This project started just two months ago. Therefore no technical accomplishments and progress presented.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.2** for technology transfer and collaboration.

- Bringing the diverse membrane supply options in as project collaborators should provide DOE with a good platform to compare pathways, and may reveal synergistic applications.
- Pursuing diverse membrane types will not likely develop close collaboration among the champions of those diverse suppliers.
- Plans for coordination between GTI and several commercial materials suppliers sound good. As noted above, should work toward a plan where we don't have to go to full scale membrane module development before significant testing of membrane flux in presence of expected impurities.
- Good project team, but who is integrating the work efforts of each member?
- Should take into account membrane work being carried out by other institutions.
- Good broad-based group of collaborators if all participate.
- Using membrane reactors. Could collaborate with PD3 on technology if IP concerns do not cause problems.
- Multiple organizations are involved in this development.
- Good quality collaborators.
- Project would benefit by involvement of an industrial gasifier vendor (GE, Shell, ConocoPhillips, . . .) by providing access to extended operating experience at scale and possibility to expose materials to gasifier conditions early and for extended periods. (Admittedly coal and coke are different than biomass, but they do provide an opportunity for extended exposure.)
- Teaming with Arizona State University, NETL, Schott North America, and Wah Chang is good.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.4** for proposed future work.

- The project proposers have laid out a reasonable plan, but it is too early to determine follow-on research.
- As noted above, need to focus on membrane tolerance to impurities before making ANY plans to integrate with a gasification reactor.
- Scope of work should be given as a timeline.
- Why is the economic analysis being done in Task 2? Should be done throughout project and especially at beginning to drive research.
- The "road map" slide is not a roadmap. Following this, the project team is bound to get lost.
- Good plan. Program just started.
- Presentation contained few fall-back pathways – Q&A indicated the investigators are aware of some options (such as relocating membranes downstream of reactor, near cyclones) but apparently haven't analyzed process consequences.
- Membrane materials development (metal, ceramic, and composite membranes) will be done by the sub-contractors.
- GTI will incorporate the membrane module inside a biomass gasifier and carry out the test.
- It appears there is disjoint between the membrane development work going on at ASU and what GTI presented.
- Chance for success is low.

Strengths and weaknesses

Strengths
- FB gasification of biomass is an important emerging renewable energy source for the electric utility industry. Co-production of H_2 is an obvious place for H_2 research to be.
- Project addresses reasonable spectrum of initial membrane choices.
- Single stage reforming-shift-separation is reasonable starting assumption.
- It is good that this concept will be tested.
- Good project team.
- GTI’s known strength is gasification.
- Three alternative membrane technologies are being evaluated. Maintain focus in these areas.
- CO_2 capture potential.
- Membrane H_2 separation – membranes' potential advantages in SMR, WGS and gasifier reactors are significant and well understood.
- Reasonably good teaming arrangement.
- GTI's persistence to continue this concept.

Weaknesses
- Lab-scale (2" diameter) FB reactor as first in-reactor test cell is unlikely to yield same results on biomass at scale.
- Plan for addressing spectrum of feedstocks, or alternatively reasons for selecting a given biomass feedstock for this work, was not given.
- No detailed plans.
- Flowsheet not sufficient.
- Cost analysis should guide research.
- Membrane survival with dust/ash/char/tars clogging and alkali condensation a concern.
- No partner that understands membrane manufacture.
- Scale-up/scale-down of fluid bed units is difficult. Need to address this. Would anyone invest in technology based on size of unit gathering data?
- Project has been delayed by funding availability.
- Experience has taught at least one industrial gasifier vendor to test materials to be used in gasifiers *in situ* as soon and as long as practical. The opportunity exists for this project to encounter unexpected, unfavorable performance relatively late in the project.
- Challenges in developing a practical H_2 membrane solution are substantial — historically, few practical successes have been achieved in much milder environments than gasifiers.
- Position of membrane within the biomass gasifier is of great concern. Will it really shift the WGSR equilibrium?
- Efficiency of the proposed concept is missing.

Specific recommendations and additions or deletions to the work scope

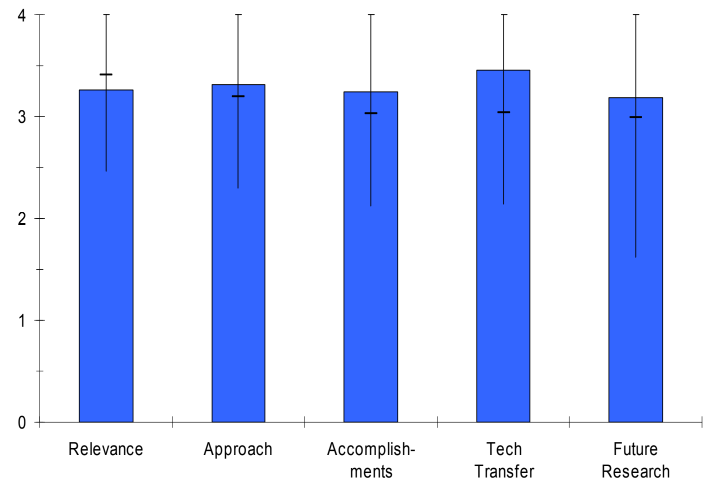
- Cost analysis should precede additional R&D.
- More focus on needs for membrane development / mfr / contaminants, etc.
- Understanding scale-up for mega-scale units.
- Characterize biomass characteristics that work well /not well in this type of process.
- Include a go/no-go after Task 2.
- Identify what (species and their level) will foul each type of membrane.
- Chances for success are low.
- Ask GTI about their earlier work on this particular concept.

Project # PD-07: Carbon Molecular Sieve Membrane as Reactor for Water Gas Shift Reaction
Paul KT Liu; Media & Process Tech.

Brief Summary of Project

Media and Process Technologies has developed a membrane with high efficiency conversion capable of converting the CO created during on-site hydrogen production to 99+% as opposed to approximately 70% through the use of high temperature shift alone. The high conversion is a result of the new membrane configuration. A pilot test of the new membrane in a reactor will be conducted at the end of FY 07. Process simulation; hydrogen production economic analysis; design, simulation and economic analysis of the polishing step to achieve 99.999% purity will follow in preparation for conceptual design of the field test unit.

Overall Project Score: 3.3 (8 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

- Viable concepts for combining reforming/shift/separation unit processes are vital to a long term, low system cost.
- The contractor is focusing on the development of microporous membranes which are an area of interest to DOE for hydrogen separation.
- The presentation was extremely vague on the specific targets required by DOE. No cost estimates were provided. In addition, no clear flux targets were provided – just a vague comparison to metallic membranes – which appears low and in odd units.
- The work does address process intensification – which is a key area of DOE interest.
- The temperatures being considered are low – 200+ degrees. There should be consideration to get this a bit higher – maybe into the HTS range.
- Goals of this program are well aligned with the DOE Hydrogen Program.
- Interesting work, but not a critical piece of the puzzle for hydrogen success. Conventional WGS works pretty well and isn't overly expensive.
- Hydrogen purification/separation is a critical component of hydrogen production.
- Developing reactive separation membranes that do not use expensive materials (such as Pd-alloys) can have very significant payoff in overall hydrogen production costs.
- Need to address the effect of non-infinity separation factors for microporous membranes.
- A membrane within the water-gas shift reactor should benefit hydrogen production pathways that use reforming.
- Carbon molecular sieve membrane as reactor/separator for water-gas shift reaction will be developed in this project. Streamlining unit operations involving CO conversion/H_2 separation and purification is very relevant to overall DOE objectives.
- Developing a small, more cost effective (capital and operating) hydrogen clean up system is relevant to the DOE objectives.

Question 2: Approach to performing the research and development

This project was rated **3.3** on its approach.

- Well thought out and described.

- The approach is reasonably straightforward and involves general testing of existing membrane materials. There is no significant novel development, for example, no new membrane materials are being developed.
- Scale-up to a larger size unit should provide valuable information.
- Catalyst testing and membrane development appear to be occurring along two separate paths. They need to be integrated together into a single development path.
- Testing of membrane performance is comprehensive with a clear line of sight to DOE hydrogen production cost targets and reliability.
- Development of a mathematical model will be critical to ultimate process design. This is a very sound and comprehensive approach to ultimate process design.
- Nice plan for success, including scale-up, pilot testing, economic analysis, safety, and end-user tests.
- Unclear what the hydrogen pressure is exiting the membrane.
- This project is using a process development approach to determine the needed hydrogen purification and reaction kinetics to meet the performance targets.
- Using TSA-based adsorption as the final polishing step offers the potential to meet the desired hydrogen purity levels.
- The target CO value should be decreased to 1 ppm CO for distributed hydrogen production for dispersing to fuel cell vehicles.
- There will be other impurity level constraints in addition to CO, for these systems that must be met for the systems to be deployed.
- A membrane within the water-gas shift reactor will improve the CO conversion and/or reduce the size of the water-gas shift reactor.
- This process produces hydrogen at low pressure which then needs to be compressed. The ultimate measure is in the cost of hydrogen, where the hydrogen is at 300 psi.
- Unclear if the presence of H_2S and water affect the membrane.
- Team will develop a reactor/separator system capable of producing 99.999% pure H_2. To achieve this goal they will incorporate carbon molecular sieve membrane with a water-gas shift catalyst and eliminate the two separate water-gas shift reactors (low and high-temperature). By removing hydrogen using the molecular sieve membrane, they will shift reaction equilibrium.
- It is a well planned approach.
- Presenter did not mention the barriers addressed in their project. This information is missing in their slides.
- The approach to generate bench scale data, generate a model, extrapolate to pilot scale, and then validate the model is standard engineering process.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.2** based on accomplishments.

- Benchtop experiments yield useful data.
- Good comparison of simulation results and test data.
- The technical progress is difficult to judge. Although actual results are alluded to and appear to be included on some of the graphs, much of the work appears to be mathematical modeling. However, it is not clear which are results produced from this work and what is from the literature. It appears that the project has been minimally funded (30%) so it is not clear how much actual progress has been made.
- The use of microporous membranes will not likely give the most effective separations. The purity and percent recovery will remain a concern and the contractor has not done a lot to improve on the situation. The separation mechanism itself will likely limit these parameters.
- Impressive testing of membrane in real-world conditions by using a slip stream from a hydrocracker that included impurities and higher hydrocarbons.
- Very good technical accomplishments such as development of a model and demonstration of a membrane in a small scale reformer confirmed by industry end user.
- Great verification of model with experimental data.
- Excellent use of analysis during project and by end-user.
- Included polishing step which shows excellent systems understanding.
- Great pilot testing plan and results; although, membrane longevity was not discussed.

- Appropriate trade-off between lower purity and higher recovery, completed with polishing.
- They have completed modeling and some experimental verification at the component level.
- The hydrogen flux at 200 to 250 C is comparable to, or better than, that in Pd-alloy systems.
- The Pd-alloy systems typically operate at much higher temperatures, yielding 20 to 50 times hydrogen fluxes; thus, comparing the performance of the carbon molecular sieve membrane at the lower temperature is not very meaningful.
- Although the presenter indicated that the carbon molecular sieve membrane material is stable, the data show significant degradation from the 3 hour values to the 100 hour values.
- The model seemed to over-predict the observed performance indicating that the model's parameters need adjustment.
- They presented good data which indicates promising results.
- Insufficient explanations and legends lead to confusion.
- Mathematical model has been experimentally verified.
- HiCON process has been developed for the small-scale reformer by the end user of this technology.
- Process optimization study demonstrated that 97-99% H_2 purity can be accomplished. This is lower than the objective of producing 99.999% H_2 purity. The team has plans to obtain higher purity.
- This project start date was October 2003. Only modest technical accomplishments have been achieved.
- The technical accomplishments to date are somewhat confusing. The stated goal is 99.999%, but reports that 97-99% clean-up was accomplished and that a non-defined adsorbent would polish the hydrogen to 99.999% with CO apparently being the principle impurity at < 10 ppm. This must be addressed.
- The <10 ppm CO target seems out of step with fuel cell targets of < 0.2 ppm.

<u>Question 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **3.5** for technology transfer and collaboration.

- Partner collaboration and contributions were not clear.
- Technology transfer and industry involvement appears minimal. There are some academic publications. The intro slides did list involvement of other partners, but their roles and contributions are not clear. It appears that the testing is primarily being conducted by MPT and the University of Southern California. The industry partners need to be more involved to ensure that the developed technology is worthwhile.
- Impressive collaboration between academia and industry; this project meets the ideal for partnership; result is the leveraging of new technology from academia (membrane) applied with an eye toward ultimate commercialization (provided by industry end user).
- Excellent inclusion of end-user!
- The project has good collaborations; academic, industry, and end-user.
- Having Chevron involved in the project is helpful to keeping a realistic check on the project's progress.
- Good combination of collaborators - include academic, manufacturer, and user.
- Good team. Team includes USC (for membranes research), Johnson Matthey (for catalyst development), and Chevron (end user).
- Seems to have good collaboration among team members.
- Working with USC, JMI and Chevron is a very good plus.
- Was consideration given to include one of the specialty gas companies (APCI, Air Liquide, BOC/Linde, Praxair)?

<u>Question 5: Approach to and relevance of proposed future research</u>

This project was rated **3.2** for proposed future work.

- Future direction is proceeding towards testing of a moderate scale membrane assembly. This appears to be an existing apparatus and testing should be straightforward.
- The testing needs to incorporate realistic gas feeds.
- Proposed future work is valuable; glad to see that it will include an economic analysis by industry end user; this ensures an objective, reality based analysis.

- Analysis should include a comparison with conventional, proven H_2 production technologies (e.g. steam methane reforming, water-gas-shift, pressure swing adsorption).
- Not a lot of future research proposed. Depends on funds availability?
- Researchers should present ideas for future research.
- Pilot-scale testing would help to obtain the data needed to validate the performance models.
- The proposed economic analysis is needed to substantiate the potential cost attractiveness of this process.
- In particular, the use of the polishing step needs more careful analysis, as the ultimate purification may add more to the cost than expected on the basis of a preliminary analysis.
- The pilot-scale testing and economic analysis are both needed.
- In FY2007, the team plans to complete pilot scale testing using a single, full-scale hydrogen selective membrane and synthetic feed to demonstrate the optimized HiCON process. End user will complete preliminary economic analysis.
- Field demonstration will be done in or after 2008.
- The above plans are reasonably good. The PI presented detailed path for moving forward.
- The future work proposed makes sense and fits in with the stated plan.
- Work to improve the effectiveness should be included.

Strengths and weaknesses

Strengths
- Good that a preliminary economic estimate of capital cost was made.
- Overall, a very good science and engineering effort.
- Straightforward test project that should be able to be completed in a minimum amount of time.
- The project has a good combination of modeling and experimental efforts.
- The project has a good combination of academic and industrial collaboration.
- A membrane can eliminate moving parts and switching valves of PSA based systems.
- A membrane will shrink the shift reactor.
- Good team.
- Good planning.
- The design as portrayed appears to be applicable for a number of merchant grade hydrogen applications and thus applicable.

Weaknesses
- Preliminary economic analysis capital cost estimate did not seem to properly include fabrication costs. Seems to be a materials summary only.
- The contractor needs to provide more details on the experimental conditions. Only limited data is provided to evaluate the work, and this makes it almost impossible to assess the actual state of the work.
- Although the presenter referred to 10 ppm CO as being readily achieved, during the Q&A it was stated that CO was at 20 to 30 ppm. It was not clear what caused this discrepancy.
- Compression energy is quite significant, particularly for compressing the product gas from 15 psig to 300 psig. This must be included in the process simulation; otherwise comparisons with alternative approaches will not be consistent.
- Not specifically a weakness, but it is not clear why the test feed gas had up to 31% nitrogen and only 44% hydrogen in the separation verification tests; this composition is reflective of ATR reformate rather than SMR reformate.
- If a PSA can remove the CO down to 0.1 ppm and a significant retentate is needed in the burner, then why use a membrane to convert CO, especially if the membrane will work only at low temperatures?
- Standard information about barriers addressed that was present in all other presentations is missing here.
- This project started in October 2003 and modest accomplishments were reported over the past three years — what are the reasons?
- What about long term durability of carbon molecular sieve membranes under process operating conditions?
- They missed on clean up – 99 vs. 99.999%.
- There is a lack of suggestions to determine the cause of the miss.

- There is a lack of a plan to correct the miss.
- The energy requirement for storage is not fully included. H_2 supplied at 15 psi not 300(?) psi.

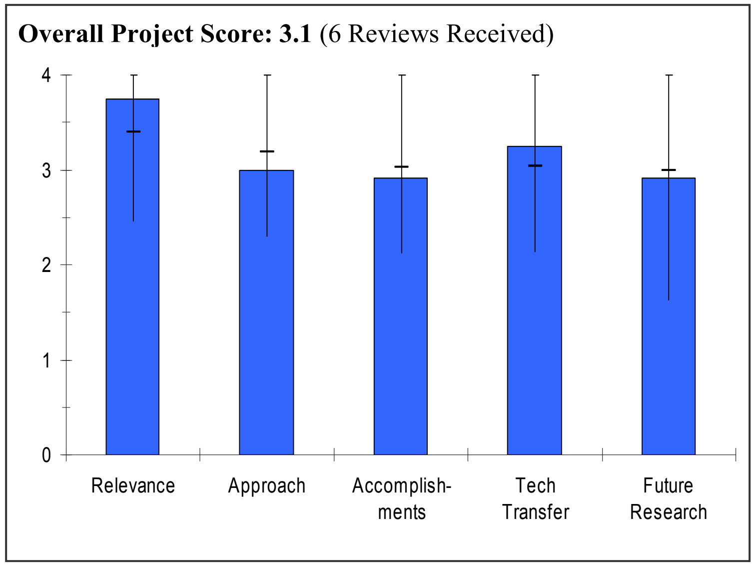
Specific recommendations and additions or deletions to the work scope

- The contractor needs to finish the work as proposed and provide some solid technical data - particularly on the reaction conditions.
- DOE needs to provide the conditions to the contractor for testing.
- Appears to be an excellent research team. Suggest DOE provide additional funds to carry this project to completion and request involvement in other R&D efforts.
- The permeate from actual reformate should be analyzed in great detail to identify all species that makes it into the hydrogen. One set of data from a pilot test shows C1 and C2 species in the hydrogen.
- Very high hydrogen recoveries are not necessary since the retentate can be sent to the burner to generate heat for the reforming reaction.
- The use of a membrane is much more effective if it can operate at higher temperatures, where the CO conversion kinetics and perhaps the permeance are even faster.
- Considerable data has been shown. These should to be evaluated closely and in detail.
- No change is needed. Continue the work.
- Investigate the escape.
- Evaluate the application of a less extensive clean-up for other merchant usage (this might free up existing facilities for the higher quality demand expected in 2015-2020 time frame).

Project # PD-08: Renewable Electrolysis Integrated System Development and Testing
Kevin Harrison; NREL

Brief Summary of Project

This project examines the issues with using renewable energy to produce hydrogen by electrolyzing water. Objectives are to characterize electrolyzer performance under variable input power conditions and develop standard testing procedures; design, build and test shared power electronics packages and controllers to reduce cost and optimize system performance; identify opportunities for system cost reduction through breakthroughs and incremental improvements in component integration focused on commercialization and manufacturability; and test, evaluate, model and optimize the renewable electrolysis system performance for both dedicated hydrogen production and electricity/ hydrogen cogeneration.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.8** for its relevance to DOE objectives.

- Renewable electrolysis supports the President's Hydrogen Fuel Initiative.
- Addresses overall program objective of hydrogen production from renewable resources. Attempts to address specific barriers related to cost, efficiency, and integration of renewable energy supplies.
- Project directly addresses the DOE Hydrogen Program goal of generating H_2 from renewable electricity.
- The project assists with system and cost optimization to advance hydrogen production from distributed and central wind electrolysis closer to the DOE cost and performance targets.
- Good effort on improving the overall system efficiency by targeting the power electronics and system integration.
- The project needs a quantification of overall average system efficiency improvement goals and timelines.
- Cost of renewable (e.g., wind electricity) energy should be used for projecting utility cost contribution in the cost of hydrogen production.
- Renewable-based hydrogen production is a very important part of the Hydrogen Fuel Initiative.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- It appears that there is limited research to reduce cost.
- There appears to be lots of modeling, but more validation is needed.
- Focusing on the overall system is good.
- Specific goals are lacking.
- Applied solid engineering approach to improving efficiency of integrated electrolyzer and performance of system seems suboptimal at low power levels, which was due to a very narrow and specific design constraint of the electrolyzer.
- Sound approach combining modeling with real-world validation; then using the model to optimize electronic control.
- Well conceived plan to ultimately maximize recovery of theoretical maximum available wind power.

- Collaborations enable access to real-world wind power generating facility.
- Design, installation and baselining component performance appears to be well executed. It is unclear if they have systematic approach for modifications made to electrolysis units.
- Using a combination of modeling and experimentation to optimize the overall system efficiency is a good approach as this is a complex system.
- Hardware-in-the-loop, as being done in this project, is an effective approach to design the power controller and electronics for this system.
- Further listing of "technical gems" in the approach is needed/should be highlighted.
- Good combination of analysis and technology development and testing.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.9** based on accomplishments.

- The progress seems modest for 3.5 years into the project.
- There is a need for more data – one hour is not impressive. With the system set up, there should be quite a bit of data generated.
- It appears that they have developed good safety procedures.
- They demonstrated that there is a lot of room to improve efficiency of wind turbine/electrolyzer combination.
- Significant progress in demonstrating systems to integrate electricity from wind to electrolyzers.
- Added benefit of demonstrating integrated H_2 production with compression and storage through collaboration with industry partner.
- Completed individual dual component baseline including stack characterization, but not a lot of rigorous testing under variable current conditions, also no simulated wind modes.
- Project appears to be in early stage of accomplishments on the experimental side, though quite some time has elapsed.
- Simulink model development and hardware-in-the-loop testing work is progressive and looks good; however, model validation data should be presented.
- Improvement in captured efficiency from Gen1 to Gen2 is impressive.
- Not clear what the impact (i.e., cost) of system performance optimization is.
- Control approach shows significant promise.
- Good progress has been made characterizing existing technology.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.3** for technology transfer and collaboration.

- It appears to be a good team and there is good team integration.
- NREL is providing valuable feedback to their partners on how to improve their products.
- HUG collaboration effort is good since it should enable rapid distribution of information.
- Close collaboration and financial support from utility industry partners. Wasn't clear from the presentation what support came from electrolyzer or wind turbine suppliers, the two industries which could best benefit from understanding how best to integrate their hardware for this purpose (hydrogen production plus grid electric supply).
- Impressive collaboration with industry and academia.
- Valuable project cost leveraging with Xcel Energy.
- Working with a number of key players in wind presents a great opportunity to share best practices from both an industry and academic perspective.
- Good collaboration between so many diverse team members.
- This project has a significant number of partners.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.9** for proposed future work.

- One of the objectives is to identify areas for cost reduction; this does not appear in the plan.
- Validation of the models using the generated data should be a goal.
- The future path builds on the past direction of engineering optimization. The plans are sound, but it is unclear why public funds are being used to do this work.
- The presentation was unclear about a number of things including: (1) their approach to electrolyzer modification for greater efficiency and optimization (e.g. higher pressure, higher temp, and ancillaries), (2) integration of power electronics for wind turbine and electrolyzer. These items are probably well thought through, but they need to be documented better.
- Proposed future research is the highlight of this project. The results from the integration of wind energy and electrolysis in several different possible configurations shall be very useful for the technical community.
- Step-wise approach, as presented, is the ideal way to move forward in testing/optimization of the complex system.
- A lot more work needs to be done with the remaining budget.

Strengths and weaknesses

Strengths
- The summary report is reportedly going to detail lessons learned and other important items.
- They are using some real world wind data in their model.
- It appears to have a well balanced team including industry, universities, and national laboratory.
- They have produced several formal reports.
- Overall relevance to DOE's technical and portfolio goals.
- Good teamwork between several partners and subcontractors.

Weaknesses
- Since they have the system built, there should be more real world data.
- This is a straightforward engineering exercise in optimization of hardware and software for commercial products.
- The project strongly needs a fuel cell and electrolyzer expert on the team.
- Lack of clarification on the targeted deliverables in terms of cost, efficiency and timelines. Just citing DOE targets is not sufficient.
- Slow progress.

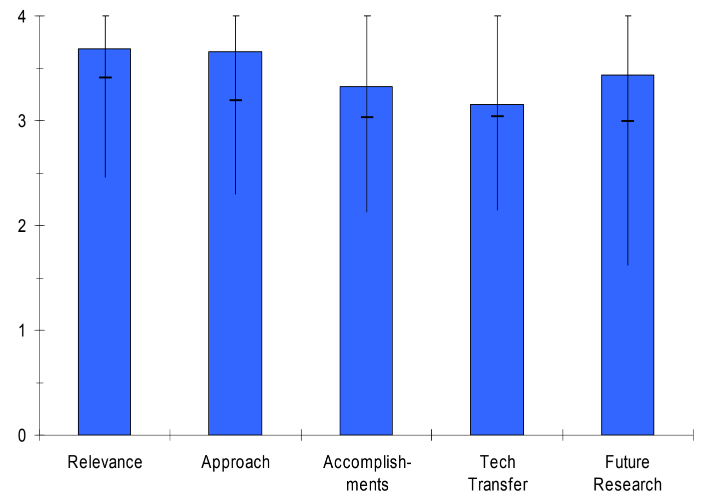
Specific recommendations and additions or deletions to the work scope

- They need to generate long term performance data.
- They should address areas of cost reduction.
- A plan to achieve the MW scale wind to electrolysis system needs to be developed. It should include the critical path (i.e. what are the highest risks to achieving the goal) and a risk mitigation plan.
- They may want to discuss this project with some refineries in Texas (Class 4 wind state) to see if the refiners have an interest in producing H_2 from a green source.
- The scope is adequate. Further additions might further delay the progress.
- The project team should determine how much the performance targets will reduce system cost.

Project # PD-09: Biological Systems for Hydrogen Photoproduction
Maria Ghirardi; NREL

Brief Summary of Project

Overall Project Score: 3.5 (7 Reviews Received)



The goals of this National Renewable Energy Laboratory project are to develop and optimize anaerobic and aerobic photobiological systems for the production of hydrogen from water and to integrate photobiological with fermentative organisms to more efficiently utilize the solar spectrum and the substrates/products from each reaction. The project is organized into three tasks: engineer a H_2-producing catalyst ([FeFe]-hydrogenase) that prevents O_2 from inactivating the enzyme's catalytic site under aerobic conditions; improve the light conversion properties of a H_2-producing anaerobic algal system by immobilizing the cells on a flat matrix; and test the ability of H_2-producing, fermentative organisms to consume algal biomass and to produce extra substrate (acetate) required for high yields of algal or photosynthetic bacterial H_2 production in a second reactor.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.7** for its relevance to DOE objectives.

- This project presents a novel approach to long-term renewable hydrogen production.
- The project is in line with DOE program objectives for hydrogen production.
- The work addresses a key technical barrier for biological production.
- This project seems to be directly relevant to the DOE Hydrogen Program for production of H_2 from biological systems.
- The proposed work is very important to the RD&D plan. These studies could be far reaching and apply broadly to a variety of biological hydrogen production strategies. For example, the goals of subtask one will contribute directly to the feasibility to utilize hydrogen producing enzymes in bio-inspired or biomimetic materials. Meeting the future energy needs of the planet will clearly require the implementation of a number of mechanisms and the NREL group and the current project is well placed to contribute emerging technologies that we probably have yet to appreciate their potential and their importance in the future global alternative energy profile. The engineering of an oxygen sensitive [FeFe]-hydrogenase is an ambitious goal but the group has provided some basis that this is possible and this is a significant contribution. These challenges for this goal are compounded by the absence of a direct selection method for oxygen tolerance, but the rational approach the group has implemented is promising and starting to produce positive results.
- The project goals are critical to the Hydrogen Initiative and fully support DOE RD&D Objectives for hydrogen production.
- Project supports MYPP long-term biological R&D.
- Project is high risk, potentially high pay off R&D appropriate for DOE investment.
- Project addresses multiple issues of proposed biological H_2 production process.
- Proposed process is a low greenhouse gas emissions process — potential exists to design process to have negative GHG emissions.
- This is assumed to be a longer term solution - the work is considered relevant.

Question 2: Approach to performing the research and development

This project was rated **3.7** on its approach.

- This project has a well-defined approach to achieve progress toward the DOE targets. Future work is also defined in the same sub-task structure.
- The subtasks for the year are appropriate to move the project forward toward meeting the objectives. However, the work appears to be open ended (no project end date is give), whereas all other production projects are finite, with defined scopes and timeframes and are fairly strictly held to DOE targets and schedules. This makes it difficult to assess the extent to which this approach will contribute to the overall due objectives a technology readiness decision in 2015.
- Speaker clearly understands and communicated that the state of the art is significantly far from performance needed for this technology to be commercially viable to meet DOE H_2 production cost targets.
- Approach was clearly stated and appears to be well thought-out.
- Impressed by the use of molecular dynamic simulation to aid catalyst synthesis.
- The subtasks all address the target technical barrier – continuity of H_2 production.
- The project is well-designed and the team has excellent experience to address the subtasks.
- The project is technically feasible and the investigators have provided key data that indicate that the project can be advanced in a timely manner.
- Although the subtasks are not discreetly integrated, each is important to the overall goals and is nicely complementary to the other funded efforts in the program.
- The project subtasks are well-focused on specific technical barriers.
- The project subtasks are well-balanced with respect to different technical barriers.
- The project subtasks are clearly designed to integrate with other research supported by the DOE Hydrogen Program.
- Approach is fairly straightforward.
- The approach presented is rational and systematic.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.3** based on accomplishments.

- Progress was described for each subtask and the project was able to obtain interim support from another source to complete work that would have been cut due to lack of funding from DOE.
- The progress toward 2010 targets was not adequately addressed. In the presentation, there did not appear to be a direct comparison for the duration target. There was no discussion of any annual milestones, decision points, etc.
- Program appears to have significant accomplishments given limited budget and funding discontinuities.
- Technology will need significant breakthroughs to meet DOE H_2 production cost targets.
- The investigators have made a clear comparison to the relevance of the proposed project to the goals of the DOE.
- The favorable performance on some indicators may suggest the DOE goals may need to be adjusted and could be more ambitious.
- For this project realistic cost and benefits estimates for this longer term solution technology is difficult to address and was not reported in the presentation.
- The group has made significant progress on all subtasks in the overall project.
- The selection or derivation of specific milestones and performance indicators was not evident; however, the progress towards specific performance parameters has been excellent. In evaluating this project as a research endeavor, the progress has been outstanding. There have been numerous publications resulting from this funding, with more in preparation.
- The demonstration of continuous hydrogen production under sulfur-deprivation growth conditions is very promising.
- The progress in computational modeling to guide experimental design of the oxygen-tolerant hydrogenase was very good, with the identification of a novel pathway for oxygen entry to the active site.

- The progress has been all the more remarkable given the reduction in FY06 funding.
- Good, considering funding.
- Good efficiency improvement from sub-task 2.
- The computation analysis appears to be yielding insight on defining next steps.
- The 25% improvement in yield was encouraging.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.2** for technology transfer and collaboration.

- The project is coordinating with other partners, but the contribution of each partner to the work was not included in the slides.
- Partners were listed and briefly mentioned, but the full extent of the collaborations wasn't clear from the presentation.
- A dedicated slide regarding collaborations would have helped.
- Program appears to be doing an excellent job in leveraging academia expertise in its work.
- The NREL group has numerous collaborations with other academic institutions.
- The project boasts strong collaborations at the University of Minnesota and the University of Illinois.
- The project does not list any industrial collaborators.
- The coordination of the work done in subtask one has been very productive and provided the basis for the design of site-specific amino acid substitution experiments.
- Most of the research is not developed to the point where opportunities for technology transfer are apparent.
- The investigators mention in a tangential fashion the use or development of proprietary materials, but there does not appear to be a coordinated, strategic plan to partner with industry for design and scale-up of the cell immobilization matrix.
- The investigators demonstrate excellent coordination and collaborations with university researchers.
- The investigators demonstrate good coordination and collaborations with international researchers.
- Good academic domestic and international collaborations.
- The collaboration with other research institutions is very good.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.4** for proposed future work.

- A timeframe for completion of the "Future Work" described in the presentation was not specified, which would have been helpful considering the fact that a project end date was not provided.
- The proposed future work is appropriate to move forward.
- "Newly identified" targets were mentioned, but it wasn't entirely clear what those new targets are.
- The group has provided a clear and rational plan for each of the three subtasks based on the past progress.
- The implementation of high throughput screening methods for identifying oxygen tolerant hydrogenases will expedite the work.
- The explicit description of clear contingencies is not addressed and the investigators could strengthen the overall plan by addressing potential outcomes more directly.
- The investigators clearly present a plan to build upon their modeling success for designing an oxygen-tolerant hydrogenase, both in the choice of using smaller residues in the channel, as well as reducing protein flexibility.
- The plan to study hydrogen yield from fermentation under sulfur-deprived conditions is a logical next step from the current experiments.
- The plan to refine the architecture of algal immobilization is good.
- Project strategy contains several alternative approaches to achieve goals.
- Pretreatment of algal biomass prior to fermentation is a good idea.
- The proposed additional work sounds rational.

Strengths and weaknesses

Strengths
- The project includes a strong computational component to complement the experimental work.
- The groundwork is laid for each of the ongoing subtasks.
- The assembled team to conduct the proposed work.
- The clear plan for the future work in addressing each subtask.
- The fundamental importance of the subtasks to the mission of the hydrogen program in general and biological hydrogen production specifically.
- The investigators demonstrate clear experimental objectives with respect to their computer simulation and modeling, and do an excellent job in closing the loop back to experimental refinement of the model.
- The tenacity of the investigators to obtain alternative funding and collaborators is to be commended.
- The proof of concept for the linked fermentation/photobiological hydrogen production system was very well-done.
- The knowledge of these investigators for the microbial and algal systems under study is well-focused towards the project goals.
- The pure long term science may pay dividends in the future.

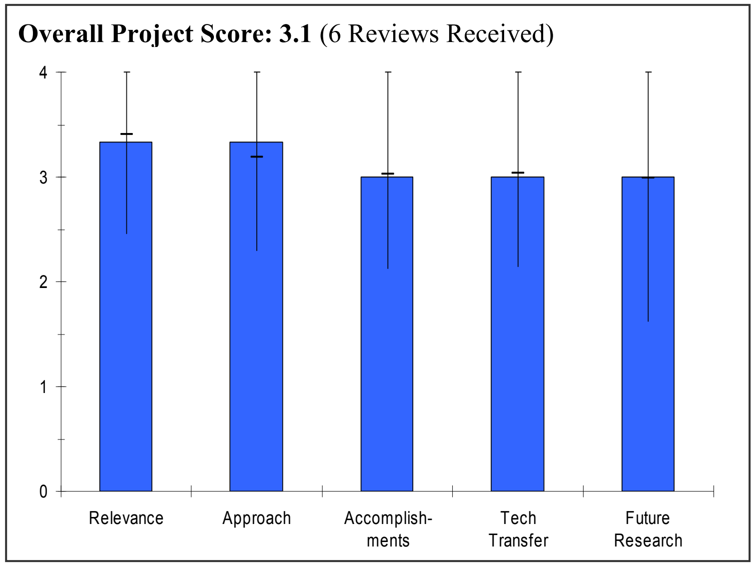
Weaknesses
- Milestones and decision points were not addressed. The P.I. also stated that the work is heading in three different directions, but there was no discussion of a down-select process of any kind to narrow the focus at appropriate times. The work is very exploratory, but the project should still have a finite scope, schedule, decision points, etc., to be fair with other production projects that are held to higher standards of definitive progress toward 2010 and 2015 targets.
- The lack of industrial interests and partnerships directly in the work.
- The lack of specific stated potential experimental outcomes and contingencies.
- It is unclear whether the mutagenesis work and modeling will be performed in parallel with the random mutagenesis experiments. There should be a clearer definition of checkpoints and cross-talk for these experiments.
- The investigators might consider whether they should continue to push for hydrogen production under algal growth conditions—given the goal of cell immobilization, they might want to try to balance algal biomass production with the microbial consortia fermentation rate. It is not clear which component contributes towards the "cost" of the entire integrated process.
- The selection of different cell immobilization matrices was not described in sufficient detail to ensure a systematic or rational choice of matrices vs. an ad-hoc, random approach. This is especially important if cost of the matrix becomes an issue.
- I do have a concern that mutating the various microorganisms may generate a bio-hazard. Are safe guards in place to address this?

Specific recommendations and additions or deletions to the work scope

- The scope should include milestones, decision points, down-select criteria, and an end date. Such open-ended research contradicts EERE's evolving focus on tech transfer, near-term commercialization targets, etc.
- None.
- You might consider working with some of the companies dealing with sewage treatment to get an understanding of how to apply this technology.

Project # PD-10: Photoelectrochemical Water Systems for H_2 Production
John Turner; NREL

Brief Summary of Project



The goal of this research is to develop a stable, cost effective, photoelectrochemical-based system that will split water using sunlight as the only energy input. The objectives are to: 1) identify and characterize new semiconductor materials that have appropriate bandgaps and are stable in aqueous solutions; 2) study multijunction semiconductor systems for higher efficiency water splitting; 3) develop techniques for the energetic control of the semiconductor electrolyte interface and for the preparation of transparent catalytic coatings and their application to semiconductor surfaces; and 4) identify environmental factors (e.g., pH, ionic strength, solution composition, etc.) that affect the energetics of the semiconductor, the properties of the catalysts, and the stability of the semiconductor.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

- The project objectives are in line with the program objectives.
- The work addresses key barriers for PEC production of hydrogen.
- The overall NREL project is well aligned with the DOE Hydrogen and Fuel Cell Initiative goals and objectives.
- Project is clearly aligned with the DOE Hydrogen Program goals.
- Speaker clearly stated the significant challenges required to compete with commercial photovoltaic/electrolyzer systems which are near-commercial.
- Good relevance and an important pathway to realize the DOE's long term objective of renewable hydrogen.
- Competes with PV electrolysis. Relative merits and demerits of this approach against PV electrolysis should be discussed.
- If this is assumed to be a longer term solution, then the work would be considered relevant.
- This activity might also compliment NASA's space exploration concepts of generating fuel (hydrogen) and oxygen from ice collected in space and on stellar bodies.

Question 2: Approach to performing the research and development

This project was rated **3.3** on its approach.

- The approach is well-defined and highly integrated with other research efforts.
- The approach is appropriate to make progress toward the objectives. The challenges and drawbacks to the different materials were adequately identified. Down-selection processes and criteria were not discussed. The work is open-ended, making it difficult to assess the degree to which this approach will contribute to the overall DOE objective of a technology readiness decision by 2015.
- The efficiency and energetics issues are relatively well addressed in the project.
- Technical barriers are clearly understood as are the targets that need to be achieved to compete with photovoltaics.
- Materials fabrication is critical – is the program leveraging with collaborators who are practicing the state-of-the-art in materials fabrication (not a criticism; but required to maximize chances for success)?

- It would appear that the ability to test large numbers of different materials is critical to project success (guided, of course, by the application of solid state physics). Are there rapid material screening techniques that could be used?
- Good approach to focusing on materials starting with PV library and modifying compositions/structures.
- Good fundamentals (e.g., lattice structure) driven approach to materials development.
- Quantification of targets for the "ideal material" appropriate and an adequate way to address the gap. Right set of test matrix for the screening exercise.
- The approach appears sound.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- Progress was described for each subtask and the project was able to obtain interim support from another source to complete work that would have been cut due to lack of funding from DOE. Their partners allowed for continuation of work despite DOE budget restrictions.
- The work is moving forward, but it's not clear what exactly they're progressing towards because the project is open-ended (no end date is given). No decision points or off-ramps of any kind were mentioned.
- Granted the program has been not adequately funded over all these years, but it indicates lack of significant progress for the project to see the PI's still talking of identifying suitable materials after more than 15 years.
- Project appears to have achieved a significant number of technical accomplishments for a very modest budget.
- Low water splitting efficiency demonstrated so far. However, the problem is challenging because of competition between conversion efficiency and the corrosion resistance of the choice of materials.
- CGS system promises high splitting efficiency but still a materials challenge in terms of fabricating such a system.
- The progress is at a pace which is to be expected for a science research project.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- The project is coordinating with many other partners who are all working together to leverage the expertise and work of each team.
- Partners were listed and briefly mentioned, but the extent of the collaborations was not clear from the presentation. A dedicated slide regarding collaborations would have helped.
- Parallel stability and durability tests of promising high efficiency materials by independent entities, perhaps by industrial partners, are needed.
- Work is clearly exploratory and far from commercialization, so it's very positive to see the significant collaboration with academia as well the solar cell industry.
- Good collaboration between diverse team members. Partnering with UNLV was a good approach to negate the effects of 2006 funding pitfalls.
- The collaboration appears to be appropriate with the state of progress on the program.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- The future plans are not well defined for FY08; however, this is likely due to the highly collaborative effort. This project has made good progress in the past and this will more than likely be continued in their future research.
- The proposed future work is appropriate to continue making progress, but it's not pointed at any specific target or materials down-selection.
- Fundamental questions should be addressed to whether the high solar to hydrogen efficiency of these III-V or I-III-VI materials would ever overcome the cost and durability issues the PI's face.

- Is there an optimum efficiency, materials cost and durability performance that need to be met?
- The establishment of some sort of a standard photoelectrochemical test protocols should also be addressed.
- Future plans slide is a bit vague on future research for 2008. Challenges to overcome and distance from ultimate goal are great; more detailed research plan is essential.
- Proposed future research is adequate to deliver on the scope of the project. The question remains on whether with the new approach the goals of the program (presumably high water splitting efficiency to compare with PV electrolysis) can be addressed.
- The proposed future research appears to be consistent with the goals of the project.

Strengths and weaknesses

Strengths
- The project has a clear idea of efficiency goals and how this concept must measure up with competing technologies.
- Well addressed efficiency and energetic issues.
- Good alignment with DOE goals.
- Good relevance to DOE's long term technical and portfolio goals.
- Good teamwork between several partners/subcontractors.
- Good (and justified) focus on fundamentals to design the new material.

Weaknesses
- No milestones, decision points, or down-select criteria were mentioned. The work is 16 years old and still going without an end date. The work is exploratory, but the project should still have a finite scope, schedule, decision points, etc.
- There does not appear to be enough emphasis on material stability and durability issues, which is critical.
- Continued work on semiconductor materials, no matter how efficient they may be under ideal laboratory environments, might not be worth the effort if they degrade under real life conditions (need industrial partner(s) to conduct real life testing).
- Lack of clarification on the targeted deliverables in terms of water splitting efficiency and timelines.
- How do the materials being researched match with the "green" and recycle requirements coming out of Europe and California?

Specific recommendations and additions or deletions to the work scope

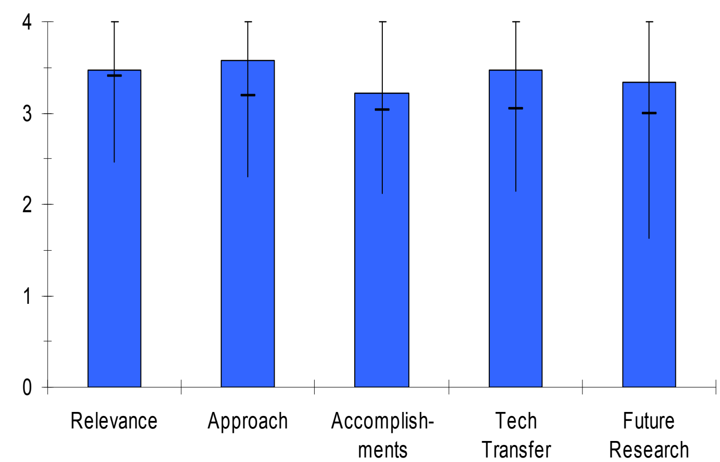
- Add to scope to look at material stability & durability issues.
- Overall, the project objectives are important in future hydrogen mix and this work should continue to be funded. However, the project needs infusion of new ideas to achieve significant gains in efficiency, lower material cost, and higher stability and durability performance.
- The scope is adequate. Further additions might further delay the progress.
- Keep track of "green" requirements. Generating a material that industry would be prohibited from using would be counterproductive.

Project # PD-11: Development of Solar-powered Thermochemical Production of Hydrogen from Water
Chris Perkins; UNLV

Brief Summary of Project

The purpose of this project is to develop solar thermochemical water-splitting routes to hydrogen production. The objectives are to: 1) identify one or more competitive solar-powered water splitting process for hydrogen production; 2) conduct experimental studies to complete quantitative selection; 3) perform numerical and experimental evaluation of solar receiver concepts for integration with thermochemical processes; 4) implement consistent methodology for comparing economic viability of cycles; and 5) demonstrate at least one potentially cost competitive solar thermochemical water splitting cycle on-sun at a small scale.

Overall Project Score: 3.4 (7 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

- Most of the project's aspects align with the DOE RD&D objectives.
- The funding level seems high for the effort.
- Producing H_2 from non-finite resources that are plentiful in America is an essential part of a sustainable hydrogen economy. Producing H_2 directly and efficiently from solar energy is an important part of this.
- Has relevance – long term potential – solar concepts do not have a record of being economical.
- In that the Program's goals include a significant amount of hydrogen production from renewables, solar-derived hydrogen cannot be ignored. This project offers an excellent opportunity to utilize this country's vast solar resources.
- The project is not taking into account the cost of delivering hydrogen from central concentrated-solar production sites, which may be remote and far away from hydrogen demand. While the H2A model can be used to calculate the central production cost, it is highly recommended that the analysis include H2A delivery analysis to determine if the viable locations for this technology result in unusual and unacceptable hydrogen delivery costs.
- Solar powered water splitting has the potential to meet the need of hydrogen production from renewables if the capital cost can be reduced. This high risk research that requires some significant R&D breakthroughs will likely only be undertaken by the federal government, so good fit.
- Good relevance and an important and interesting pathway to realize the DOE's long term objective of renewable hydrogen.
- Competes with PV and direct photoelectrolysis. Relative merits and demerits of this approach against those approaches should be discussed.
- Supports MYPP for high temperature solar thermochemical technologies.
- High risk, high payoff project appropriate for DOE.
- Low greenhouse gas emissions approach to H_2 production.

Question 2: Approach to performing the research and development

This project was rated **3.6** on its approach.

- The project approach focuses on the technical barriers effectively.

- It is good that cost is being used as a determinant in the selection of the cycle. Materials are a big issue, but this is not being fully addressed.
- Good mixture of modeling and experimental work.
- Concentrating on the very high temperature capabilities of solar concentrators is a good selection. This increases the range of possible chemical reactions, and thereby casts a wider net of opportunity.
- Consideration of potential environmental impacts in the process down-select criteria is a plus.
- Avoiding duplication of effort on the Sulfur/Iodine cycle is good management.
- Has screening and down select mechanisms – good approach.
- Much parallel work – need to down-select soon to focus funding on the best approach(s).
- See analysis (costs, manufacturability) to help in down-selecting, but balance of analysis vs. experiments.
- While this technology may be cheaper than PV/electrolysis, does the inability to co-produce electricity reduce its potential application in a future hydrogen/electricity energy sector? Also, co-production of electricity can reduce necessary storage costs. Project economics need to evaluate the impact of storage costs.
- Great work on heliostat design.
- On-sun testing is very appropriate. Glad this isn't just a lab simulation or a CFD analysis.
- Good focus and progress on electrochemical cell design.
- Pleased to hear that 30 or more experts assembled to assist in generating ideas for designs that could lead to a lower cost heliostat.
- Good collection of various solar thermochemical cycles. Overall good approach to address the gap by expanding the funnel of ideas followed by down-selection.
- Excellent efforts to build closed experimental cycles and then use observed performance as the selection criteria.
- Good combination of experiment and CFD modeling.
- Good inclusion of H2A in evaluation of cycles.
- Good risk reduction – carrying along multiple different (5) cycles.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.2** based on accomplishments.

- It appears that good progress in the experimental work has been made.
- Economic evaluation is extremely important and it is great to see that progress was made on the heliostat cost reduction. It would be good to see the cost reduction numbers validated.
- Grinding of the CdO to improve hydrogen production rates seems to require too much work for the hydrogen produced, especially considering the progress on the other candidates.
- Halfway thru the project they have made good progress.
- Screening and scoring hundreds of potential reaction cycles, they reduced the focus to a dozen cycles potentially compatible with solar concentrating capabilities.
- Five process flow sheets were downselected that offer conceivable pathways to success.
- Processes and reactor configuration options have been identified for these five. Lab-scale hardware investigations with on-sun proofs of concept have been thought through and offer reasonable chance of success for the latter half of this project.
- Good review of many thermochemical cycles.
- Considerable experimental work – lots of reactors.
- Excellent progress on down-selecting options.
- Need more information on how the 351 cycles were scored and how so many were eliminated to get down to 12.
- CFD modeling great for designing reactor.
- Good progress on doing on-sun experiments. Suggest these be integrated with analysis on system design, including storage and delivery requirements.
- Great that project is doing cost analysis with H2A. Need more info on capital cost estimation. Who is reviewing cost analysis?
- Down select and experimental testing of 5 cycles and transference of eight from a starting point of 351 is impressive.

- Slow technical progress. At this stage some of the cycles should have been ruled out by identifying the showstoppers.
- Quantification of technical accomplishment (in terms of improved efficiency) should be provided.
- Good progress and solid technical work in design of the solar receiver reactor.
- Comparison between ZnO vs. HyS costs was informative. Similar should be done for all cycles.
- Good progress in improving conversion in aerosol reactors.
- Good recognition of need for and pursuit of heliostat cost reduction.
- Good progress on reactor development for several different reactor types.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.5** for technology transfer and collaboration.

- There is a large team assembled, but it is hard to tell who is contributing what to the project. It would be useful to indicate which team member is responsible for the different aspects and tasks.
- Good progress in selecting candidate processes and conceptualizing process configurations for these diverse processes is indication of good teamwork across the spectrum of program participants.
- Keeping up with the commercially available hardware capabilities rapidly becoming available in Europe, especially Spain, is an important source of collaboration.
- Broad group of collaborators.
- Excellent team. Would be good to show who is doing what in the presentation. This was a comment from last year, which although responded to, was not incorporated into the presentation.
- Workshops on heliostat design were a great way to get expert advice and direction. Is one of the project partners going to carry out new design analyses?
- A number of government agencies as well as private industry will benefit from the ongoing fundamental material analysis.
- Good and seamless collaboration between diverse team members.
- Technology transfer appears easy once the downselected cycle and its merits have been demonstrated, because the choice of scale is adequate.
- Broad participation of academic, national lab and industrial partners.
- Workshops brought in additional expertise.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.3** for proposed future work.

- There is a great deal of work that needs to be done in a relatively short amount of time.
- There should be enough data to begin down selection and then materials development for the cycles selected.
- The team is focused well on the materials and process challenges presented by their down-selects, and is positioned to be successful in the second half of this project.
- Have a good down-select plan but need to do it and not stay in the science mode.
- Suggest systems integration field work.
- Need to provide more details about lifecycle impact of successful cycle.
- Concern remains over the costs associated with the heliostat.
- Proposed future research is adequate to deliver on the scope of the project.
- Heliostat cost reduction a big barrier to success of the project and the promised cost reduction. Strong efforts needed to achieve that (outside of the scope of the current project).
- Good continued use of H2A.

Strengths and weaknesses

Strengths
- There is a broad team with plenty of funding.
- There appears to be a good mix of modeling and experimental work.

- They are focusing on cost as a discriminator for the cycles.
- This is an important renewable energy pathway for American society's energy needs in this century. The researchers know that and have dedicated their efforts accordingly.
- The solar research facility at Sandia is well suited to perform the on-sun testing, and the team's familiarity with high temperature solar capability and limitations provides a reliable project configuration.
- Deployment of new solar trough electrical generation stations and the emergence of heliostat collector fields for central electrical station use is reducing the cost of solar components and building Solar-Thermal capability in several parts of the world. Hydrogen production based on this technology base will be a winner.
- Good understanding of chemical cycles.
- Solid approach and technical depth.
- Good teamwork between several partners/subcontractors.

Weaknesses
- They should have developed the solid particle receiver earlier to get more data.
- There are significant materials challenges that have not been addressed particularly for the higher temperature operation.
- At this stage, it seems the team is focused on too many cycles.
- The team seems reluctant to down select to a top 1-3 cycles and focus their resources on them.
- While concentrating on the very high temperature capabilities of solar-thermal technology makes good strategic sense, progress in developing practical process hardware for the Sulfur Iodine process that is compatible with CSP is not being pursued.
- High temperature materials issues are the apparent major barrier to development of practical process hardware for the selected cycles. Despite its focus on very high temperature cycles, this project is constrained to select from existing materials rather than develop new ones compatible with the temperatures and reactant environment.
- Strong reliance on Heliostat cost reduction.

Specific recommendations and additions or deletions to the work scope

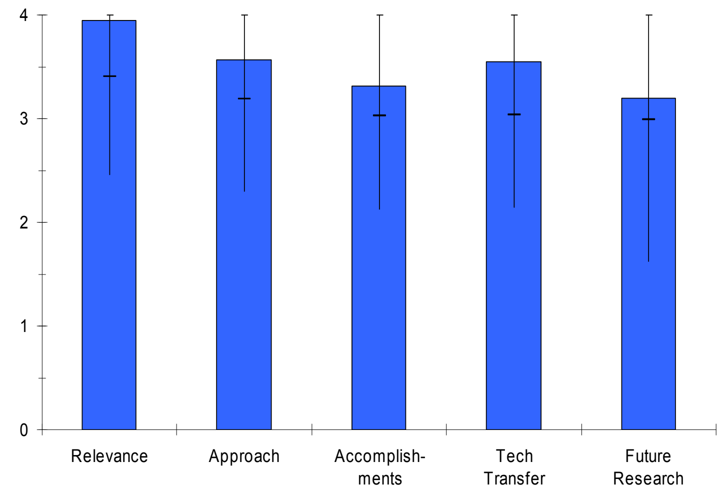
- It is recommended that they down select to 1 or 2 cycles.
- It is recommended that they need to focus more on materials development.
- While the use of H2A will "likely" conservatively cover costs of parasitic process losses, it’s reasonable to have the researchers consider specifically the possible energy losses due to materials handling to support the process concept. This may be particularly important in evaluating acceptability of reactor efficiency and material recycle ratios up and down a tower.
- Heliostat cost reduction is possible and would help the economics of these processes, but pursuing those reductions lies outside the scope of this project, I believe. If heliostat cost reduction is necessary to meet project economic targets, identify the reductions needed.
- Practical hardware configurations for solar powered H_2 production with the Sulfur-Iodine process should be designed by this team as soon as the nuclear energy based project team shows successful closed loop operation and can make process design information available.
- Much better analysis efforts.
- The scope is adequate. Further additions might further delay the progress.

Project # PD-12: Hydrogen Delivery Infrastructure Options Analysis
Bruce Kelly; Nexant Inc.

Brief Summary of Project

The objectives of this analysis are to: 1) refine technical and cost data in H2A Component and Scenario Models to incorporate additional industrial input and evolving technology improvements, including significant data additions and delivery system storage analysis and optimization; 2) explore new options to reduce hydrogen delivery cost, including novel carriers; 3) expand H2A Component and Scenario Models to include new options leading to Version 2 models; and 4) provide bases to recommend hydrogen delivery strategies for initial and long term use of hydrogen as a major energy carrier.

Overall Project Score: 3.5 (6 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **4.0** for its relevance to DOE objectives.

- Understanding delivery options and costs will be critical to understanding hydrogen production and delivery infrastructure.
- Breadth of delivery options is necessary.
- The project objectives are right in line with DOE objectives.
- For delivery analysis, critical barriers are addressed.
- Focused on key elements of delivery cost.
- The data collected in the project moves DOE closer to providing a robust H2A model that can (and likely will) have global reach. This is a critical tool for analyzing the costs claims for other DOE funded programs.
- Project well aligned MYPP delivery analyses.
- This project appears to be dead on with the activities to support the Hydrogen Fuel Initiative.

Question 2: Approach to performing the research and development

This project was rated **3.6** on its approach.

- Hydrogen production system considerations should be included in minimum storage requirement optimization. For example, on-site production systems will not necessarily have 100% availability. What considerations have been given to maintenance schedules when determining that only 0.3 days storage will be required?
- Appropriate not to place too much emphasis on currently unknown alternative delivery options.
- Although geologic storage is certainly interesting, optimizing an infrastructure that appropriately considers location and feasibility is an entire research project in and of itself.
- The approach is very thorough, very detailed, and appropriate for meeting project objectives. The analysis includes examination of many key variables that must be considered for different delivery options.
- Looking at many pathways.
- Modeling approach which gives DOE understanding of costs of all options.
- Giving inputs to H2A which is key cost modeling system.
- The collection of information from industry sources will be helpful to industry; however, it would have been useful to see some of the actual station designs that resulted from the new cost and dimension inputs for storage and compression.

- Objective approach.
- Demand data obtained from industry is crucial to provide realistic representation of system performance requirements.
- This approach is very rational and appropriate.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.3** based on accomplishments.

- Project continues to make significant progress, although there appears to have been some scope growth over the last year. It is important to focus first on the most mature and understood technologies for the initial optimization. Too much is unknown at this point about some of the higher risk options, such as carriers and geologic storage.
- The project appears to be on track. A significant amount of work has been done over the past year.
- Project milestones were not adequately addressed in the presentation.
- Many small accomplishments which add up to excellent H2A delivery model costs.
- Much data — very useful in understanding options.
- For $2 million dollars I would expect to see the actual improvements to the model demonstrated. Perhaps this will be part of next year's update. Also further explanation is needed around the level of maximum storage for worst case demand period (July 4th on a Friday). Seems counter intuitive that it would be only 1/3 of a day's need. Probably worthwhile having a special session with Energy company employees who actually work on optimizing fuel supply chain to stations. These individuals probably do not reside on the tech teams.
- Very good progress developing models and developing requirements.
- The accomplishments listed to date appear impressive and are timely.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.6** for technology transfer and collaboration.

- Good diverse team.
- Project participants were listed, but the extent of the various collaborations were not adequately addressed in the presentation. A dedicated slide to this would have helped.
- Good, broad team.
- H2A work some of best collaborative work in DOE portfolio.
- As a robust H2A model will have global reach, the potential contribution is high. Actual reports based on analysis results are needed for a full appreciation of the contribution.
- Project has good national lab and industry (gas and petroleum) representation.
- The collaboration is appropriate and diverse.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.2** for proposed future work.

- Would be useful to consider hybrid systems for managing peak demand cycles for non-pipeline-fed stations. Instead of optimizing station design around July 4, what happens if it is optimized around a more average summer day? Can peak be met with delivery from a central plant?
- In addition to delivery strategies, it would be useful to have recommendation on areas where there are gaps in current technology. For example, in the refueling site design, steps up in compressor size had an obvious impact for peak/average flow considerations.
- Although I recognize that assumptions on permitting and siting costs have to be made and that those costs for similar fuels are the appropriate starting point, it would be useful to include more variability (e.g., significantly higher costs) in this parameter for the sensitivity analysis and design optimization.
- The proposed future work is appropriate to advance the work toward the project objectives.
- Modest work for future.

- Work should be declared a success and funding stopped.
- I think greater emphasis should be placed on the current delivery models to make sure that they are as sound as possible. For instance what would a forecourt design look like with the new data? How would a centralized plant and distribution pipeline be designed for optimization?
- The proposed future work appears to be consistent with the reported activity to date.

Strengths and weaknesses

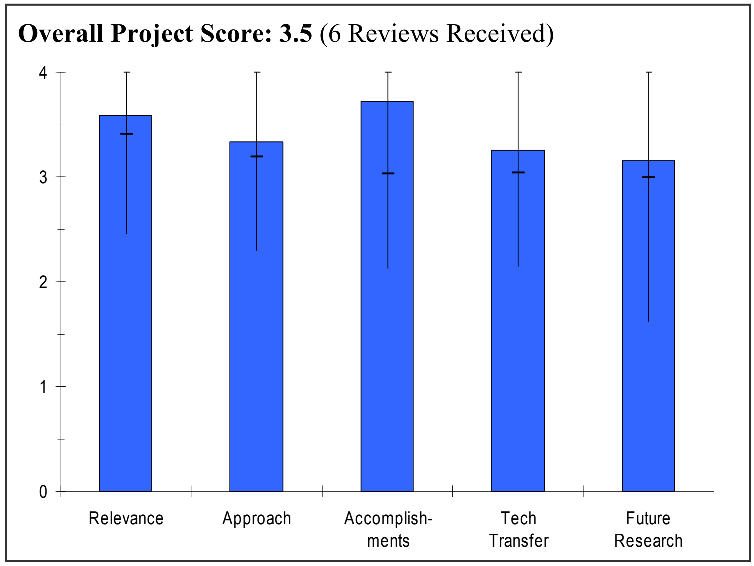
Strengths
- Team brings in a lot of industrial expertise, as well as strong modeling and analysis capabilities.
- Many collaborators.
- Excellent team play.
- The work to date reflects the current state of technology well.
- The work will be helpful with estimating the economics of the process.

Weaknesses
- Perhaps considering too many options and venturing into areas where the error bars are significant. Focus first on the known technologies.
- The effort is 70% complete, but it does not appear that even a preliminary guess as to the leading options has been formulated. This is a minor weakness because rankings and recommendations are included in future plans. Still, a preliminary estimate of leading options as soon as possible would be valuable because it could help identify R&D priorities for the next few years.
- No system to get current feedback on total costs. By this, I mean estimate – get true final construction and owners costs and then change model.
- H2A is incorporated in several models already (Hypro, Hytran, etc.) a written management of change plan that highlights how and when these other models will adopt the changes would be helpful.
- The work does not seem to address issues related to contamination of the fuel during transport and storage.

Specific recommendations and additions or deletions to the work scope

- Minimize emphasis on more advanced delivery options.
- Not knowing how service station demand data was aggregated, I'm not certain of reliability of 0.3 day storage oversize. It differs significantly from a rigorous, but much more limited (3 station) simulation study and from station oversizing currently practiced by at least one oil company. If further service station study is performed, it would be useful to learn rules Chevron applies to size stations – which should consider not only demand, but other system factors (e.g., distribution disruption factors) some of which might apply to H_2 distribution.
- Evaluate potential sources of contamination from the well to wheels and factor in the cost of maintaining the fuel quality.

Project # PD-13: Fundamental and Modeling of Pipeline Hydrogen Embrittlement
Petros Sofronis; U. of Illinois



Brief Summary of Project

The objective of this project is to come up with a mechanistic understanding of hydrogen embrittlement in pipeline steels in order to devise fracture criteria for safe and reliable pipeline operation under hydrogen pressures of at least 7MPa and loading conditions both static and cyclic (due to in-line compressors) for the existing pipeline steels and to propose new steel microstructures.
It is emphasized that such fracture criteria are lacking and there are no codes and standards for reliable and safe operation in the presence of hydrogen:
• There are no criteria (codes and standards) with predictive capabilities;
• Pipeline steels may be dangerously susceptible to fatigue failure in the presence of hydrogen.
The Illinois mechanism-based approach will:
• Develop design criteria to be used for codes and standards for safe and reliable operation;
• Avoid unnecessary repairs and shut-downs by minimizing unnecessary levels of conservatism in the operation of pipelines;
• Reduce capital cost by avoiding conservatism.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.6** for its relevance to DOE objectives.

- For a viable H_2 economy, hydrogen embrittlement must be understood and strategies to mitigate it must be developed. This project is developing a mechanistic understanding of the embrittlement problem. It is not clear that it should be funded by the production and delivery group. It may be more applicable to the Codes and Standards group.
- Hydrogen pipelines remain the most cost-effective means for delivering hydrogen over wide areas. Understanding materials issues is key to understanding materials, operational, and permitting requirements.
- Although this project does not address the economics of pipelines, it does help to address the DOE safety and reliability objectives for transition pipelines.
- Pipelines and hydrogen embrittlement is a key barrier to hydrogen infrastructure and transportation issues.
- The results from this work shall feed effectively into codes and standards development and also to some extent in identifying appropriate material/design for hydrogen storage.
- This project's objective is to come up with a mechanistic understanding of hydrogen embrittlement in pipeline steels in order to devise fracture criteria for safe and reliable pipeline operation under hydrogen pressures of at least 7 MPa. Fracture criteria for hydrogen pipeline is missing and this project tries to look into it and therefore there is very good relevance to overall DOE objectives.

Question 2: Approach to performing the research and development

This project was rated **3.3** on its approach.

- The approach is good considering the funding level.

- Model validation is required; however, the low funding level my prevent this. Maybe the industry partners would be willing to validate the model as part of their cost share?
- Modeling effort is very good, but is unclear how adequately potential intensified interactions are being addressed. For example, what is the effect of multiple cracks and how does proximity influence this?
- Fully-reflecting the impact of defects and impurities will be challenging.
- The morphology studies of used pipeline material are quite helpful in understanding the proposed degradation mechanisms.
- Combined modeling and analysis of hydrogen transport and materials failure is the right approach to address the problem of hydrogen embrittlement.
- Strong focus on fundamentals and measurements to feed into the model that will allow for development of predictive tool to predict failure criteria.
- Impressive breadth and depth in establishing the mechanism and solution approach for predicting failure of hydrogen induced crack propagation.
- Development of simple design criteria for failure is a good target.
- Tension experiments to identify macroscopic plastic flow in pipeline steels – very useful.
- Permeation experiments to identify diffusion characteristics – needed to understand crack growth mechanism.
- Experiments to determine stability of crack propagation to assess catastrophic failure scenarios.
- Development of a mechanistic model to establish failure criteria with predictive capabilities – very important to establish codes for hydrogen pipelines.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.7** based on accomplishments.

- Considerable work has been accomplished.
- There has been a lot of modeling efforts; however, experimental data to validate the models is required.
- Very strong preliminary effort within the available funding.
- Given that funding has been inconsistent and could have been a key barrier to progress, their completion of the permeability measurements and piping characterization studies really demonstrate a very high level of commitment to the work and program.
- Solid progress in model development, validation, measurements and predictive capability.
- Effort of the project team is exemplary and accomplishments easily outdistance the amount of funding provided to date.
- Significant progress for small and intermittent funding.
- Slide #20 "Accomplishments vs. Project Milestones" is an excellent one. All the milestones were met. Hats-off to the PI for doing a lot with very little funding. Glad to see this type of work is funded by OHFCIT.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.3** for technology transfer and collaboration.

- There are some ties with industry.
- Large number of presentations and publications
- Good breadth of partners identified.
- Looks to be a nice mixture of industry and the national labs. Still I am unclear about the full role of Air Liquide and APCI. Are they just a used pipe supplier or are they integrally involved in information and project design exchange?
- Happy to hear willingness to work with ASME B31 pipeline working group.
- Good collaboration with ASME in terms of establishing the appropriate factors of safety for hydrogen pipelines. This is highly needed.
- Need to lay-out a plan for future technology transfer and codes and standards development.
- Strong collaboration within delivery working group and with international delivery organizations.
- Used the Oregon Steel Mills steel for their initial experiments.

- Already looked at the inclusions in the steel structure used by Air Liquide.
- Good partners from industry and national labs (ORNL and Sandia).

Question 5: Approach to and relevance of proposed future research

This project was rated **3.1** for proposed future work.

- Model validation is needed. Perhaps they can compare the model to industry provided data since the funding levels are low?
- The research plan does not include studies of mixed use pipelines, which is the more likely scenario. The impact of the cycling should be investigated.
- Would benefit from more in-depth discussion of the design for fracture testing experiments.
- Would be nice to better understand the international connection and benefits to the project.
- Proposed future research is adequate to meet the stated objectives of the project.
- Quantification of targets will be useful in assessing the merits of proposed future work.
- Future work is good, but could be broadened to consider fatigue studies. Need to work with delivery working group to determine proper test to be carried out and threshold properties to be achieved.
- The future plans given in slides #21 and #22 are very good. PI will measure diffusion characteristics of pipeline steel samples provided by both Air Liquide and Air Products. He will determine the uniaxial tension flow characteristics in the presence of hydrogen. In collaboration with Sandia, the PI will carry out fracture testing. PI has a long term plan to continue this work.

Strengths and weaknesses

Strengths
- The PI appears to be using a sound approach and modeling.
- It appears that there are good partnerships with relevant companies.
- Good focus on non-uniform materials.
- Outstanding technical leadership provided by the PI.
- Solid partnership and team execution.
- Developing strong fundament materials basis.
- Strong background in fracture mechanics.
- Availability and training of graduate students and post-docs.
- Complete understanding of the pipeline materials problems.

Weaknesses
- Model validation is lacking, however, the PI definitely would like to validate the model. Perhaps, industry partners can provide data or validate the model?
- The project is not examining the effects of impurities or swings in pressure.
- This project is of great interest to industry for many applications in addition to the President's Hydrogen Initiative. Yet, the contractor cost share is relatively low.
- Multi-fracture and impurity interactions will be challenging. This is not so much a weakness of the project, rather a challenge that may be difficult to fully address.
- It will be worthwhile to set up a qualification test based on the results of this project at a pilot scale where such a pipeline is tested at an appropriate scale in the expected cyclic conditions, and failures are verified.
- Need stronger collaboration with industry (e.g., AIR LIQUIDE) to utilize lessons learned with existing hydrogen pipeline infrastructure.
- Does not contribute to screening/evaluating current pipeline materials. Modeling and experimentation under ideal conditions need to expand to real work gas conditions pipes may see and include mixed or trace contaminant affects on fracture.
- Seems the mechanical properties are measured on flat samples. How will the properties correlate with tubular samples?

Specific recommendations and additions or deletions to the work scope

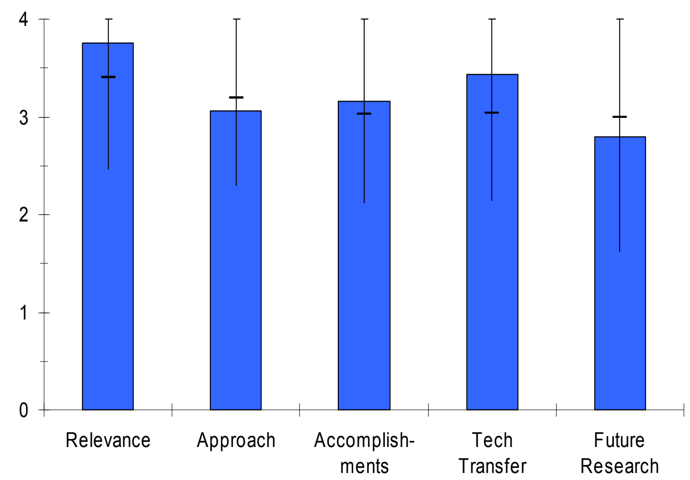
- Fully funding this project would significantly improve its impact.
- This project should be of great interest to industry. The industry cost share should be higher.
- The project should address the effects of impurities (water, CO, CO_2, sulfur ...) that may be included in the gas.
- The project should address the effects of how cycling of either the gas composition or the gas line pressure affects the pipes. For example, changing the gas in the pipes from natural gas to hydrogen and back or using the pipeline for not only delivery, but for storage with its resultant pressure swings.
- It would be good to know how the use of the hydrogen transport model with Kinder Morgan progresses as a test to the models reliability.
- Recommend to continue the project as is to establish the failure criteria but further emphasize on creating an interface to assist in establishing factor of safety and codes and standards development.
- Future scope might include doing similar analysis for off-board storage at different pressure and establish failure criteria under those conditions.
- Impact of impurity and their concentrations is also an additional future scope that shall be considered.
- Study the effect of inclusions.
- Model for other gases such as Hythane and NG.
- Study the effect of moisture and trace impurities (such as sulfur and chlorine) in the hydrogen gas going through the pipeline.

Project # PD-14: FRP Hydrogen Pipeline
Barton Smith; ORNL

Brief Summary of Project

The overall objectives of this project are to: 1) reduce the cost of hydrogen transport from central and semi-central production facilities to the gate of refueling stations and other end users to <$0.90/gge by 2012; and 2) investigate the use of fiber-reinforced polymer (FRP) pipeline technology to transmit and distribute hydrogen and achieve reduced installation costs, improved reliability, and safer operation of hydrogen pipelines. Objectives for fiscal year 2007 are to: 1) demonstrate integrity of FRP pipeline during hydrogen exposure; 2) assess hydrogen leakage in existing liner materials; 3) assess joining methods for FRP pipelines; and 4) determine integrated sensing and data transmission needs.

Overall Project Score: 3.2 (5 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.8** for its relevance to DOE objectives.

- Addresses the key element of pipeline cost (welding, materials, embrittlement) by coming up with a new groundbreaking technology.
- The project is clearly relevant to DOE's objectives of identifying low cost, safe and reliable approaches for hydrogen transmission via pipeline.
- High relevance due to cost and performance of existing pipeline systems.
- Applications for transmission and distribution.
- Since instrumentation can be integrated into manufacture and installation, very cost effective.
- The work to date is extremely relevant to the hydrogen initiative.

Question 2: Approach to performing the research and development

This project was rated **3.1** on its approach.

- It is unclear how adequately supply and demand interactions for fiber-reinforced polymer materials have been addressed. Cost assumptions are likely overly optimistic.
- Need to ensure that effects of weathering in the presence of hydrogen are adequately addressed.
- Need to ensure the effects of impurities on pipeline integrity are adequately addressed.
- Good technical approach, but more effort needs to be funded to assume success and determine if FRP systems could be economically better than current systems. Some work but more needs to be done.
- May need more "contractor" input as they evaluate sensor and joining technologies.
- Although some ASTM test methods were listed, the accelerated ageing test appears to be steady state. What happens with pipe performance over time when pressure and temperature are cycled? Is a year long enough for accelerated ageing testing? The principle should provide an exhaustive list of tests to be performed on the RFP pipe along with expected outcomes.
- Current material is commercial; this program is more characterization than R&D.
- Material systems are critically needed and address one of the largest barriers.
- Due to funding issues, this activity needs to be accelerated to provide DOT characterization of pipeline safety.

- The research to date has been focused on one composite pipeline material, which makes sense because it allows for the generation of an evaluation methodology.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.2** based on accomplishments.

- Reasonable progress within available funding.
- Progress limited by funding – good progress considering funding.
- Given that very little funding has been provided the level of effort to understand the economics and potential of FRP pipe is impressive.
- Progress was limited by funding.
- Good initial data on hydrogen permeation.
- Progress is about where it should be based on schedule and budget.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.4** for technology transfer and collaboration.

- Good partnership with pipeline supplier, but might benefit from partnering with pipeline users and/or standards development bodies (e.g. ASME).
- Good collaborators with other researchers and industry.
- Pipeline working group is a good team.
- The project includes industry and academic participants. However I do think that they should make the effort to discuss their experimental design in detail with the scientists at U of Illinois to see if Dr. Sofronis et al. may be able to assist in developing a predictive model of failure modes under varying environments. U of Illinois may also learn from this project. Perhaps this is happening via the pipeline working group.
- Good collaboration.
- Focused on using existing manufacturing technology.
- Provides manufacturer a means to improve existing technology for oil and gas industry.
- The collaboration is not as broad as I would hope. Collaboration with API, ASME, ASTM, CSA, CGA and SAE would have been expected.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.8** for proposed future work.

- Would benefit from more detailed discussion of performance testing parameters and how this will be incorporated into economic analysis.
- Weak future plans – maybe this is due to shortage of work so far.
- Needs to propose work that gets FRP pipelines to the cost target.
- Good evaluation of codes and standards needs.
- I believe the plan could be made more robust through greater engagement with hydrogen gas suppliers. Would be good to have their input on the reasonableness of the experimental design and the economics.
- Proposed work is important to determine if instrumentation and joining will hold up to prolonged exposure.
- Accelerated aging studies must be performed on liners and formed joints.
- The proposed future activities are consistent with the goals.

Strengths and weaknesses

Strengths
- Good identification of alternatives to conventional pipeline materials.
- Big step-out possibilities.
- Good team.

- Good approach to reducing cost of installation.
- This project addresses an escape in the present activities.

Weaknesses
- Unclear how adequately pipeline integrity testing has been addressed.
- Inconsistent funding.
- Need risk assessment on damage tolerance.
- Field manufacture needs to be verified for pipe sizes over 4 inches.
- The project is presently limited to a single material. Evaluation of other similar composite and plastic materials is needed.

Specific recommendations and additions or deletions to the work scope

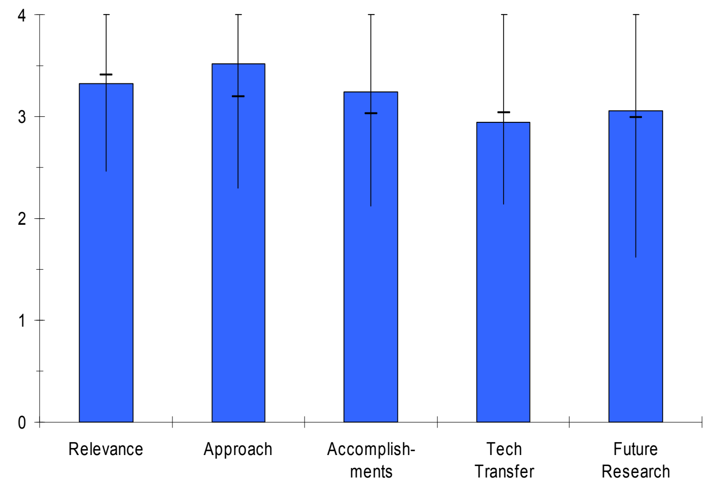
- Could they do more, faster if they had more money? As pipelines are becoming more important to the transition, this project should probably be elevated in terms of priority.
- Provide funding to complete the study in a timely manner.
- Collaborate with SAE and ASME on other non metal, common plumbing materials that should be evaluated.
- Collaborate with ASTM and API on any material specifications for these materials which need to be revised or generated.

Project # PD-15: Scale-up of Hydrogen Transport Membranes for IGCC and FutureGen Plants
Doug Jack; Eltron Research Inc.

Brief Summary of Project

The objectives of this project are to: 1) develop high-throughput, low-cost H_2 separation system suitable for application with coal-based synthesis gas, including improved tolerance to contaminants (S, Hg, etc.) and enabling cost effective capture of CO_2 for sequestration; 2) select candidate mechanical configuration (tube vs. plate; metallic alloy vs. cermet) considering cost, performance, and manufacturability of membrane and system; 3) scale up membrane and system from 0.45 lb/day of H_2 using lab gases to 220 lb/day in coal-derived syngas; 4) integrate membrane design into a 4 ton/day H_2 production unit; and 5) determine optimum process design and cost and compare vs. other systems.

Overall Project Score: 3.3 (7 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

- Good presentation, relevant to FutureGen program including sequestration.
- The project aligns well with the President's Hydrogen Fuel Initiative by developing a critical element needed for commercial hydrogen purification, i.e., the scale-up of hydrogen transport membranes for FutureGen and IGCC applications.
- CO_2 capture in line with DOE goals.
- DOE targets for high flux and selectivity met.
- Exceeds DOE goal for CO_2 capture considerably.
- The development of a technology for hydrogen separation from fossil fuel combustion exhaust gases is at the heart of a sustainable transfer to a hydrogen economy. It could not be more in line with America's demand for future energy.
- Low cost, higher performing membranes are needed as an alternative to PSA.
- Carbon sequestration is a major challenge due to the amounts of gases needed to be processed.

Question 2: Approach to performing the research and development

This project was rated **3.5** on its approach.

- Company has solid background in materials.
- Scale up steps are appropriate – progress made to skip a step.
- The technical approach follows five major steps to meet the objectives of the project. These steps include the scale-up of the membrane system through two stages (220 lb/day and 4 ton/day) and culminate in an optimum process design and cost comparison.
- The technical approach also includes an identification of the business development challenges associated with the project and strategies to address these challenges.
- Built on past work to identify a preferred material of choice for the membrane that will be used in the scale-up tests.
- Proposed acceleration of scale-up is viable.
- Excellent summary of objectives and approach.

- Excellent methodology and approach, economics will drive the adoption of new technology.
- Approach is good.
- Development schedule could be more aggressive.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.2** based on accomplishments.

- Elton has already met or exceeded 2010 targets.
- Material development efforts can compete with existing materials.
- Improved CO_2 capture with their approach.
- Good scale-up of catalyst deposition.
- Achieved the first scale-up step under full WGS conditions.
- Improved the knowledge base of the impact of membrane materials and preparation techniques on degradation and embrittlement.
- Developed necessary process engineering and economic tools for system optimization.
- Developed a membrane system that met/exceeded the 2010 DOE targets for flux and selectivity.
- Constructed a 1.3 lb/day unit that will now be used for collecting data for life cycle analyses.
- Promising membrane pretreatment methods developed that can improve membrane performance.
- Membrane system meets 2010 DOE targets for flux.
- PI could provide more details on decay but did indicate their system performs better than Pd.
- 5% improvement compared to Selexol.
- Warm gas cleaning shows promise.
- Avoidance of hydrogen embrittlement and hydride formation is very important. The investigators noted this but gave no details on how project is addressing these two issues.
- Already meets 2010 targets for hydrogen separation. Would consider adjusting targets for the project.
- Lifetime/durability testing needs further work.
- Developed their own new materials.
- Level of intellectual properties.
- 97/98% capture from exhaust stream – Excellent work.
- There is some concern that as the project advances to larger development scale, it may encounter some of the same problems as other, similar past projects. Companies have been involved in a number of similar technology programs, but approach seems mired in the same problems as ITM, SECA, etc.
- Manufacturing and sealing for joints have not been addressed in material selection 3.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.9** for technology transfer and collaboration.

- Technology transfer/collaborations not adequately addressed due to time, N/A?
- Would have liked to spend some time on this area, given how close they are to "commercialization."
- Would like to hear more about patents that have come out of this research.
- The project has three partners, all of whom appear to be well qualified to participate in a project of this nature.
- It is unclear if any of the participants will invest in the effort to commercialize the concept or if their level of participation will remain on a fee-for-service basis. Eltron appears to be aware of this and is seeking a commercialization partner.
- Good collaboration between partners.
- Coordination among collaborators.
- Intellectual property issues appear unresolved.
- Market penetration and commercialization issues appear unresolved.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.1** for proposed future work.

- Schedule looks reasonable, based on logical steps and accomplishments to date.
- The proposed future research effort hinges largely on the identification of a suitable commercial partner. No contingencies or optional pathways have been discussed to address project risks, including that mentioned above.
- Focused R&D plan culminating in the design, construction, and testing of a 4 TPD unit.
- Consider adding partner for catalyst coating.
- Determine mechanism of failure. Collaboration with a materials characterization group would be valuable.
- Key areas of future work are defined as a result of the previous work.
- Working towards addressing lifetime/durability issues, for example hydrogen embrittlement.
- Scale up is planned into future work.
- Economics look favorable.
- Appears "business as usual".
- Project could be more aggressive or market driven.
- If current industry demand required technology it might be developed faster.

Strengths and weaknesses

Strengths
- Met or exceeded DOE goals.
- Company seems to understand technical issues such as embrittlement.
- Good that Eltron looks at manufacturing and not just technical components.
- Promising approach for membrane scale up.
- Developed model for membrane performance that can minimize the number of tests needed.
- Results for cermet membrane vs. Pd membrane appear very promising.
- Gantt chart for future work provided.
- Large amount of intellectual property being generated; 3 patents already plus another 4 in processing.
- Clear leadership working with academic and industrial institutions.
- Good technical team.
- High performance hydrogen transport membrane family identified.

Weaknesses
- Put dimensions on reactor slide to show relative size.
- Put dimensions on tube design slide to show relative size.
- Address key technical HTM issues identified so that they do not become show-stoppers.
- Conclusive tests will be needed to address the potential of hydrogen embrittlement.
- Design life of catalyst (for hydrogen disassociation) is 5 years. If catalyst fails, the entire membrane assembly will have to be recoated and reassembled.
- No management push to drive technology development faster or propose more aggressive solutions.
- Marginal improvement.
- No independent assessment of risk or cost.
- Not clear how they will fund 220 lb / day unit and test by end of 2009.

Specific recommendations and additions or deletions to the work scope

- The project produces a by-product stream of CO_2 with about 5 percent hydrogen. Economics of capturing this 5 percent of hydrogen may be dictated by the CO_2 sequestration techniques. There might be an opportunity for a CO_2 sequestration project to team up with this project to address this matter perhaps through joint funding.
- A thorough study of the mechanisms of hydrogen-related failure is needed. What is the mechanism? Hydrides and embrittlement?
- Very good project, which is meeting 2010 goal. However, the level of spending is very high for one element of the hydrogen community, when compared to other DOE funded projects. Eltron is currently generating lots of patents, will this hinder future development of carbon capture and storage?

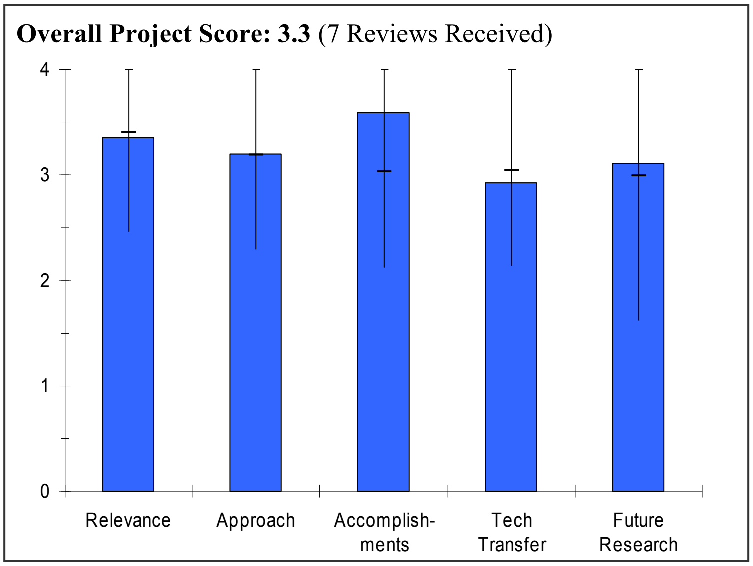
PRODUCTION AND DELIVERY

- I have scored the project highly for its technical merits, but it is my professional opinion that funding should be split between different parties so that no one organization holds the intellectual property rights.
- Cost share should have been higher.

Project # PD-16: Cost-Effective Method for Producing Self-Supporting Pd Alloy Membrane for Use in the Efficient Production of Coal-Derived Hydrogen

Kent Coulter; Southwest Research Institute

Brief Summary of Project



The objectives of this project are to: 1) develop a process methodology for the cost-effective manufacturing of thin, dense, self-supporting palladium (Pd) alloy membranes for hydrogen separation from the mixed gas streams of coal gasification processes; 2) reduce Pd membrane thickness by >50% over current state-of-art, and show potential to meet DOE 2010 technical targets; 3) demonstrate viability of using large-area vacuum processing to "engineer" a membrane microstructure that optimizes hydrogen permeability, separation efficiency, and lifetime; 4) demonstrate efficacy of large-batch and/or continuous roll-to-roll manufacturing of membrane material with performance and yields within pre-defined tolerance limits; and 5) demonstrate separation efficiency of thin palladium membrane in commercial-type fuel processor using mixed gas streams.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.4** for its relevance to DOE objectives.

- Able to down select to appropriate membrane.
- Concept of Pd-alloy separating membrane is definitely relevant.
- However, use and production of free-standing film may not be readily translatable as a practical, low-cost option.
- Good work for basic manufacturing explorations (hence, high relevance); but not too useful for large-scale, high-volume, low-cost, production.
- The project aligns well with the President's Hydrogen Fuel Initiative by developing a critical element needed for commercial hydrogen production, i.e., a self-supporting Pd-alloy membrane for hydrogen separation.
- Strives to address the following areas: Defects (high yield, large area), Selectivity (>99.9%), Flux (>100 scfh/ft2), Cost goal (<$1500/ft2), all of which are barriers identified by DOE.
- Supports the Hydrogen Fuel Initiative.
- Targets barriers related to defects, selectivity, flux and cost.
- Separation of H_2 from mixed gas streams is necessary for several pathways.
- Highly relevant to DOE objectives.
- Very appropriate to DOE goal.

Question 2: Approach to performing the research and development

This project was rated **3.2** on its approach.

- Looks like a good approach.
- Good solid work to understand basic process manufacturing; but the weaknesses are: free standing thin films must be integrated into functional modules which requires a multi-step process!
- Not clear if project addressed cost of module manufacturing.
- The technical approach follows a staged 3-year plan, 2 years of which have been successfully completed.

- A no-cost extension has been granted to complete the remaining tasks.
- There are no concerns with the proposed approach to reach the stated objectives.
- Hydrogen gas used for reported flux results.
- Should use synthetic mixed gas or actual coal driven synthesis gas.
- Clear goals.
- Cost realistic and cognizant.
- Excellent steady year by year progression in size and quality of membranes.
- Magnetron sputtering is a very appropriate strategy to maintain Pd/Cu alloy composition during deposition.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.6** based on accomplishments.

- SRI understands membrane "manufacture".
- Achieved flux goals.
- Collaborated with Idatech back to DOE on scaling techniques.
- Unique way to estimate cost of Pd.
- Given that it's basic work on films, work shows solid progress in reduction of thickness and good permeation results; but sensitivity numbers cannot be defended if there are no real mixed gas experiments.
- Somewhat disappointed that real module data is not available, which means good current results could be lowered when the films are subsequently incorporated into modules.
- Achieved the first scale-up step under full WGS temperature and pressure conditions.
- Improved the knowledge base of the impact of membrane materials and preparation techniques on degradation and embrittlement.
- Developed necessary process engineering and economic tools for system optimization.
- Completed most of the planned accomplishments for Year 3.
- Membrane composition for Pd concentration identified.
- Down selection to batch process is a logical determination.
- Increased size of membranes produced.
- Exceeds DOE's target performance.
- Achieved 4-micrometers thick Pd film, pea-hole free, on oxidized Si wafer. Range of ~3 to 12 micrometers.
- Met H_2 99.95% quality goal.
- Impressive Pd based film that is pea-hole free.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.9** for technology transfer and collaboration.

- Good work based on Colorado School of Mines and SWRI activities.
- Good acknowledgement of partners.
- Clearly, good cooperation between SWRI and Colorado School of Mines.
- Collaboration with IdaTech is not truly evident at this stage due to delays in module testing.
- Paper highlights SWRI's strengths and capabilities and Colorado School of Mines solid manufacturing approaches.
- No clear definition of issues with IdaTech Is it more a serial transfer of materials rather than active partnership?
- The project has only one for-profit partner, who is likely to be the sole entity to spearhead the commercialization effort. Delays with partner caused the project to require a no-cost extension.
- There is no distinct assurance that the project will move to commercialization once DOE funding ends.
- Sealing of foil on full scale design reviewed by DOE. Now it is time for implementation.
- Palladium cost $35 out of $45 using industry established model indicates program is going in the right direction.
- Collaboration between industry and university for ternary work.
- A good balance of team members.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.1** for proposed future work.

- Milestones clearly developed and communicated.
- Unlike other papers, speaker did not give rationale for choice of ternary alloy components. No references are made to other work on ternary alloys, or why or how they will approach the ternary work.
- Appears to want to continue same vacuum deposition approach without defending why this is best for ternary systems.
- The proposed future research effort involves two additional partners – Carnegie Mellon University and TDA Research. The plan is to utilize an iterative modeling, rapid fabrication, and testing approach to develop and demonstrate <5-micron thick ternary Pd-alloy membranes.
- Reducing cost as mentioned for thin films to $10 range would be a major cost reduction.
- Plan to go to ternary alloys 74 Pd-24 Cu4M.
- Approach and relevance is appropriate.

Strengths and weaknesses

Strengths
- Good presentation, hit all the appropriate points
- Produced thinnest membranes that exceed DOE targets.
- Good presenter – answered questions thoroughly.
- Solid pedigree based on Dong Wong's work.
- Reasonable approach for binary systems and vacuum deposition is time-honored and proven for other high-volume film processes.
- Uses a novel, scalable vacuum deposition method to fabricate free-standing Pd-alloy hydrogen separation membranes. The vacuum deposition method allows for tight control over the layer composition and thickness.
- Produced <3 micron, and 110 in^2 membranes and verified their performance, which was acceptable.
- Competent team of a commercial partner (IdaTech), Colorado School of Mines, and a new partner of CMU.
- Final tests under more aggressive conditions to develop new ternary alloy formulations with increased durability.
- Preliminary cost calculations show the cost of membrane is $10/ft^2 more than the current price of Pd.
- Gave credit to foundation work at Colorado School of Mines.
- Has aggressive commercial partners.
- Development of (3-5 micron) self-supporting PdCu films.

Weaknesses
- Pd-Cu alloy and stoichiometric choices not unique or innovative.
- No extension to practical modules (work delayed).
- No mixed gas results to verify separation efficiency.
- No clear analysis of solubility effects versus diffusional parameters.
- All tests completed so far were performed using pure hydrogen. No synthesis gas mixtures (simulated or real) were used in the evaluation. It is unclear if the membrane's efficacy will be retained when gas mixtures are used.
- Full-scale prototype tests not completed with project 95% complete.
- Sputter deposition techniques are sophisticated.
- Magnetron deposition times.

Specific recommendations and additions or deletions to the work scope

- Need better defense of future work on ternary alloys – why certain choices? And would similar process work on ternary systems? And would that be meta-stable status?
- Definitely need mixed gas data and reduction to practical modules to get more realistic cost/ft^2 estimates.
- None. Project is near completed and is under a no-cost extension.

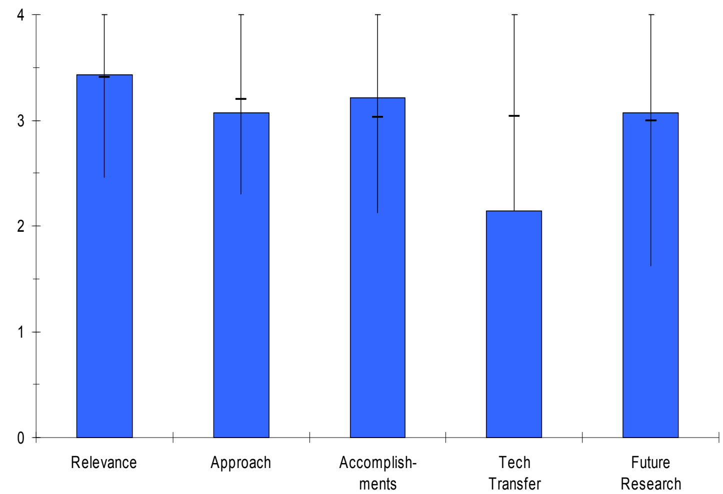
- Complete full-scale prototype testing.
- Should cross reference H_2 sensor work to understand the performance/lifecycle issues of annealing per the characterizations of catalytic coatings.

Project # PD-17: Advanced Water Gas Shift Membrane Reactor
Suzanne Opalka; United Technologies

Brief Summary of Project

The objectives of this project are to: 1) identify through atomistic and thermodynamic modeling a suitable Pd-Cu tri-metallic alloy membrane with high stability and commercially relevant hydrogen permeation in the presence of carbon monoxide and trace amounts of sulfur; and 2) identify and synthesize a water-gas-shift (WGS) catalyst with a high operating life that is sulfur and chlorine tolerant at low concentrations (0.004 atm partial pressure at 42 atm total pressure) of these impurities.

Overall Project Score: 3.1 (7 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.4** for its relevance to DOE objectives.

- Work is highly relevant and innovative to combine WGS catalyst with H_2 separations system.
- Atomistic and thermodynamic modeling efforts are very thorough and well-explained.
- Objectives well-specified.
- The project aligns well with the President's Hydrogen Fuel Initiative by its effort to address two critical elements needed for commercial hydrogen separation, i.e., the development of a robust Pd-Cu tri-metallic alloy membrane with high stability and hydrogen permeation rate and to identify and synthesize a water-gas-shift (WGS) catalyst with a high operating life that is sulfur and chlorine tolerant.
- Lower cost conversion of syngas to H_2 and CO_2 key to producing H_2 from coke oven gas.
- Handling of sulfur is an important issue.
- Mathematical modeling appears to be outstanding.
- Clear goals, objectives, and analysis provide great direction.
- Results show excellent progress.
- A well thought out project that addresses DOE goals.

Question 2: Approach to performing the research and development

This project was rated **3.1** on its approach.

- Crosses over with fuel cells.
- From design to modeling to analysis – the approach is well done and systematic.
- Solid presentation of modeling results and correlation with measurements.
- Good understanding of both solubility and diffusional effects on permeation through designed structures.
- The technical approach involves computational modeling of membranes coupled with experimental verification of predicted results. This approach has significantly shortened the time to develop, test, and optimize the preferred catalysts for the said purposes.
- Several new alloy combinations have been identified via modeling. Their hydrogen solubility, permeability, and diffusivity appear promising, but have yet to be verified by experiment.
- Sound approach using modeling thermodynamics followed by testing. Avoiding mixed phase regions identified.
- The approach was very clear but not enough mention of cost relative to performance.
- At this stage, not enough emphasis on exponentially integrating WGS catalyst with PdCu membrane.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.2** based on accomplishments.

- Appears appropriate work.
- Able to downselect ternary alloy.
- Impressive progress integrating computations and correlations with basic experiments.
- Good cross-correlations with data from other sources.
- Solid understanding of meta-stability of systems.
- The technical accomplishments and project progress are up to date and on track.
- Two Pd-Cu-transition metal alloys and WGS catalysts have been selected and are ready for durability and optimization studies.
- Good agreement obtained between experimental results and modeling predictions.
- Several new alloy combinations have been identified via modeling. Their hydrogen solubility, permeability, and diffusivity appear promising, but have yet to be verified by experiment.
- Theoretical work on solubility and phase separation complete and PdCu membranes - PdCu alloys selected.
- Work on catalysts complete.
- Much higher H_2 diffusivity achieved by focusing on Pd-Cu B2 body centered cubic alloys.
- Phase transitions for two transition metals - denoted as J6 and G5 – tested and addition of transition metal G5 broadens B2 phase field while maintaining H_2 solubility.
- Very good progress and accomplishments.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.1** for technology transfer and collaboration.

- Did not really discuss this area in detail.
- Collaborations were not well explained during the presentation.
- Unclear what the responsibilities were of each partner.
- Once the 1500-hr test is completed and the final report is forwarded to DOE, it is unclear whether the concept will be commercialized.
- Most of the work is focused on modeling, so whether it will be attractive to investors at the termination of the project is uncertain at this point.
- Good capable team..
- Did not appear to be any special collaboration outside UTRC.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.1** for proposed future work.

- Program almost completed.
- Appropriate with respect to durability testing, but not very clear what steps follow after durability testing.
- A 1,500 hr test remains to be completed. No time period was provided as to when this would be initiated.
- Future testing worthwhile in particular stability testing of alloys and shawny throughput of integrated system.
- WGS catalyst family has been identified and will be tested.
- Direction for future work was very clear and compelling.

Strengths and weaknesses

Strengths
- Able to downselect catalysts.
- Systematic, well-presented and explained project
- Clear articulation of why downselected materials were selected.
- Good fundamental grasp of the processes and architecture.

- A good blend of modeling and laboratory verification. This will prove useful to minimize the number of experimental tests that have to be run.
- The development of the WGS reaction catalyst and the hydrogen separation membrane provide some synergy toward the production of hydrogen from coal. By removing the hydrogen in situ, the equilibrium limitations of the WGS reaction are overcome.
- Sound technical approach.
- Detailed mathematical modeling.
- The perspective of a large company.

Weaknesses
- Spent more time on first slide and did not cover all main points on slides which possessed good information.
- Presenter did not thoroughly cover material on slides.
- Need to explain and account for CO_2 interactions via experimentation as well as modeling.
- Need durability test data.
- There is some concern that the hydrogen separation catalyst and the WGS catalyst developed by this process may only be tolerant to sulfur and chlorine concentrations that are too low for actual operations. The targets are set so low that precleaning of the syngas may be warranted.
- Although the combination of the WGS reaction and the hydrogen separation step can be viewed as process intensification, the project does not address some of the other issues associated with this combination, such as catalyst poisoning by the excess CO_2 remaining in the reactor.
- The WGS catalyst is to be developed by both modeling and experimentation, but the tri-metallic alloy for hydrogen separation is limited to only modeling. It is unclear how useful the end product will be.
- Cost unproven compared to state of the art over a full cycle.
- Not much indication of relevance to the other people's work and attention to cost goals.
- Have not yet zeroed in on key integration experiments.

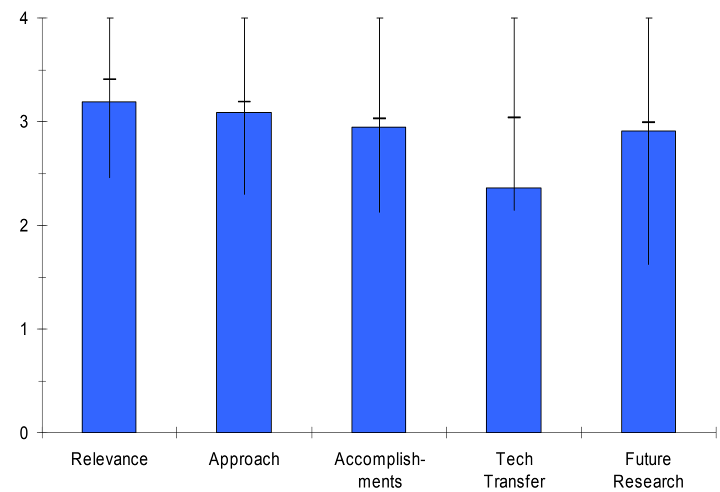
Specific recommendations and additions or deletions to the work scope

- Need more clearly defined scope of future activities beyond durability testing.
- Need scale-up to live-testing where CO_2 effects could be determined.
- Include both modeling and experimental verification for both the WGS catalyst and the tri-metallic alloy for hydrogen separation.
- In addition to Pt-based catalysts, it is suggested to test cheaper Fe-based WGS catalysts.

Project # PD-18: The Integration of a Structural Water Gas Shift Catalyst with a Vanadium Alloy Hydrogen Transport Device

Thomas Barton; Western Res. Ins. & U of Wyoming Res. Corp.

Overall Project Score: 3.0 (8 Reviews Received)



Brief Summary of Project

The key to a commercially scaled device that integrates metallic hydrogen transport membranes and water gas shift catalyst will be a catalyst with high compressive strength and no friability and a practical low cost method to attach the membranes to structural alloys. The objectives of this project are to: 1) develop a structural water gas shift catalyst capable of withstanding compressive forces; 2) develop vanadium alloy hydrogen separation membranes for fabrication of devices by brazing; and 3) integrate the WGS catalyst and metallic membranes into a device and test under gasifier conditions.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.2** for its relevance to DOE objectives.

- Relevant to DOE program.
- The project aligns well with the President's Hydrogen Fuel Initiative by its effort to address two critical elements needed for commercial hydrogen separation, i.e., the development of a low-cost vanadium alloy hydrogen separation membrane and a structural WGS catalyst, which unlike typical WGS catalysts are not friable powders, but can withstand high compressive forces.
- The use of vanadium, which is a lower cost metal compared to palladium, might help these membranes to meet the DOE's cost goals.
- Reduced WGS cost supports the H_2 Fuel Initiative.
- High compressive strength requirement for WGS catalyst with no friability dependent on reactor design.
- Integrated WGS and H_2 separation on a structural support many have a variety of applications and may be scaled down to small systems.
- It appeared to have a very limited scope and difficult to see how it was connected to other projects.
- Relevant for the production of hydrogen through improved catalysts using the water-gas shift reaction.
- The project assumes vanadium-based hydrogen transport membranes are the solution. This may be premature.

Question 2: Approach to performing the research and development

This project was rated **3.1** on its approach.

- Good exchange of information to share results with general public.
- The technical approach involves four tasks starting with the preparation of a monolithic ceramic or impregnable substrate and a brazable vanadium membrane that will be integrated and tested under coal gasification conditions.
- First three tasks are near complete. The final testing with a gasifier is yet to be done.
- There do not appear to be any inherent flaws with the approach.
- Structural WGS catalyst to integrate with membrane technology.
- Focus on fabrication for making a device.
- Brazing of membrane to tube for manufacture.

- Cost analysis of monolith versus impregnated substrate.
- Highlights practical issue of developing a device.
- Can what is learned be applied to other work?
- Use of a structural WGS catalyst and a vanadium-alloy H_2 membrane is a practical, economical approach.
- Not much connection to barriers.
- Very limited data.
- Goals are not clearly outlined or defined.
- May lead to more durable and longer-lived catalysts.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- Prepared a new water-gas shift catalyst and incorporated it into a structural water-gas shift ceramic material.
- Demonstrated vanadium alloys with excellent brazing characteristics for fabrication into membrane devices.
- Fabricated equipment for testing the integration of membrane and catalysts combinations under bottled gas and coal gasification environments.
- Cerium additions of 2% look promising.
- 15% alumina optimum.
- Analysis of vanadium alloy properties to optimize H_2 transport and brazing completed.
- A system has been assembled that can clean a slip stream of particulates, condensate, sulfur, and mercury.
- Identified materials and fabrication process to construct test reactor.
- Optimized the composition of the Fe-Al-Cr-Cu-Ce WGS catalyst.
- Identified alloying additives that improve H2 transfer and brazing properties of vanadium.
- Some progress but not much data or clear description of progress.
- Data indicates that good progress is being made.
- Question whether 80 hours is a long enough test under gasifier conditions to show viability of concept.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.4** for technology transfer and collaboration.

- Good collaboration with university.
- Once the tests with the working gasifier at WRI are completed, the project is silent on regarding any discussion on continuing efforts and eventual commercialization.
- Industry / University collaboration.
- Does not feature as a strength but they do have a small coal gasifier for testing.
- Not much indication there was any collaboration.
- Little explicit mention of outside collaborators.
- Needs to push collaboration with one of the other contributors

Question 5: Approach to and relevance of proposed future research

This project was rated **2.9** for proposed future work.

- Project almost complete; some tasks fully completed.
- The 80 hour testing with WRI's gasifier on Powder Basin coal has already been initiated in April 2007.
- Investigate use of Ce.
- Next steps will depend on test results.
- Tests with gasifier using PRB coal are just beginning. They should be completed.
- Did not clearly outline future goals and expected directions.
- Only the briefest mention of further research and that is mainly of commercialization paths.
- Approach is appropriate.

Strengths and weaknesses

Strengths
- PI was good presenter.
- The project if successful, will lower capital costs by using a lower cost metal and help meet 2010 or 2015 program goals.
- Identified elements that are potentially positive to both hydrogen transport performance and brazing performance. While other elements with favorable transport characteristics may exist, their brazing performance is less desirable.
- Practical issues of materials fabrication addressed.
- Small device constructed that can be tested and replicated.
- The use of low-cost membranes and catalysts is refreshing.
- Appears to yield a better catalyst.
- Showed that brazing is a good way to attach catalyst, but unclear if this is new information.
- Good insights into vanadium alloy brazing being developed.

Weaknesses
- Should include scale on photos on slides.
- Some alloying elements beneficial to hydrogen transport will interfere with brazing of the membranes to structural alloys. This will require some trade-off analyses and optimization studies.
- Highest activity and stability has been shown for a catalyst with 75Fe-15Al-8Cr-2Cu alloy blend with small amounts of CeO_2, but producing high surface area monoliths of this catalyst series may be problematic due to sintering at higher operational temperatures.
- Project investigators could expand partners to address catalyst issues.
- No test results presented of integrated device yet approach suitable for small systems. How would it scale up to coal gasifier which is expected to be very large?
- Believe that someone else will optimize an alloy compatible with this technique.

Specific recommendations and additions or deletions to the work scope

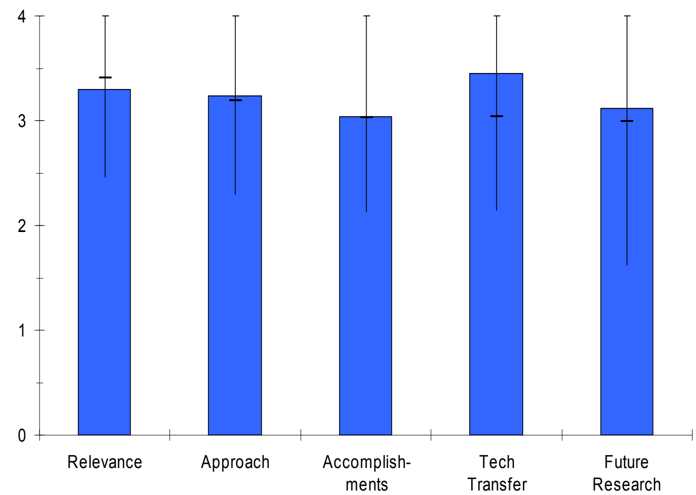
- The project is 80% complete with a planned end date of Dec. 2007. The proof of the project is based on the outcome of the tests conducted with a working gasifier at WRI, but brazing problems and hydrogen embrittlement could become potential issues.
- Include remaining needs for research in the project's final report.

Project # PD-19: High Flux Metallic Membranes for Hydrogen Recovery and Membrane Reactors
Robert Buxbaum; REB Research & Consulting

Brief Summary of Project

The project objective is to find a base metal replacement for palladium ($470/oz) and for the principal investigator's own sandwich membranes for use in hydrogen purifiers and membrane reactors with the following properties:
• Stable at 350-400 C;
• 100% selectivity like Pd;
• $100/ft^2 vs. $3000/ft^2;
• 50 scfh/ft^2 UHP H_2 at ΔP=200psi;
• 15+ life, no embrittlement.

Overall Project Score: 3.2 (6 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

- Relevant to DOE work to develop cost-effective membrane.
- The project is aligned with the President's Hydrogen Fuel Initiative by its effort to help meet cost targets for membrane materials used for hydrogen separation.
- There is some concern that the project is more focused on producing hydrogen from methanol rather than hydrogen from coal.
- Lower cost membranes with increased flux supports Hydrogen Fuel Initiative.
- 15-year life, while not a direct HFI goal is highly commendable.
- Testing with methanol reformer does not seem to be well aligned with current reforming activities.
- Innovative and creative approach.

Question 2: Approach to performing the research and development

This project was rated **3.2** on its approach.

- Seems appropriate for work at level of involvement.
- The project effort is to find a base metal to replace palladium (currently at $470/oz) that will be stable at 350-400 C, demonstrate a 100% selectivity like Pd, cost range of $100/ft^2 vs. $3000/ft^2, 50 scfh/ft^2 UHP H_2 at ΔP=200psi, and demonstrate a 15+ year life without embrittlement.
- There do not appear to be any inherent flaws with the overall approach, but whether the end goal is achievable.
- Base metal membrane with Pd on surface to dissociate H_2 on surface.
- B2-intermetallic material allows for thinner or no coating of Pd which would lead to lower costs.
- Tubular membrane approach with 15 year lifetime/durability is impressive.
- The focus is on B2-ordered alloys in which vanadium is one of the elements.
- The B2 alloys still face embrittlement issues under H_2 environment.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- Great slide on year-by-year accomplishments shows progress made.
- Identified failures as well as successes.

- Identified and evaluated about 60 alloys, some having over 100 times the permeability of Pd and costing only 1/100 times as much, but they embrittle in an H_2 environment.
- Some intermetallic alloys, like NiTi show some promise, but require further development.
- Exceeded the performance goals set for membranes in 2005 and 2006, i.e., selected alloys and achieved test flux of 51scfh/ft^2 at 44psi.
- Interesting point that 12% storage of hydrogen is possible in methanol/water liquid carrier.
- Identified elements with higher H_2 permeability than Pd.
    - Aim for B2 alloys to be ductile and stable with less cost than Pd–Cu alloys.
- Identified two alloys with comparable permeability to Pd.
- Identified the need for long life of material for commercial applications.
- Brazing-scatter approach to testing is crude, but effective.
- The use of B2 alloys is an interesting and different approach. No real hydrogen transfer data at this point.
- Good progress to date.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.5** for technology transfer and collaboration.

- Good selection of partners, good leveraging of funds.
- The presentation does not describe any plans for continuing efforts and eventual commercialization.
- The PI did not mention if his company will commercialize the outcome of this project.
- Excellent collaboration between industries, university and government laboratories.
- Very strong collaborations with partners.
- Good team put together.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.1** for proposed future work.

- Project is 50% complete.
- Good thorough approach.
- Plans are to improve alloys for high flux with no embrittlement, fabricate and test membrane and membrane reactor, and confirm that behavior matches flux, cost, and durability goals.
- Identified alloys not useful for hydrogen separation that could have other potential market applications.
- Reduced embrittlement of alloys.
- Embrittlement testing of brazes.
- Some work should be focused on how the membranes/reactors can be scaled up for larger applications.
- Test membranes/reactors on fuels other than methanol.
- Good approach.

Strengths and weaknesses

Strengths
- Good follow on activity from SBIR phase 1 funds (leveraging).
- Good presenter who offered thorough explanations.
- Great "show and tell" and good use of visuals.
- The project if successful, will lower capital costs by using a lower cost metal and help meet 2010 or 2015 program goals.
- There is a possibility that some of the developed alloy combinations that failed to meet the requirements for hydrogen membranes might find applications elsewhere.
- Targets commercial application.
- Use of methanol feed eliminates sulfur contamination issues.
- Good collaboration between project partners.
- Interesting idea.

- The B2 alloys show great promise in the areas of cost reduction at comparable flux and selectivity to those of Pd membrane.
- Good collaborations with universities and national labs.
- Highly creative project team which will lead to new novel membranes of interest for DOE.

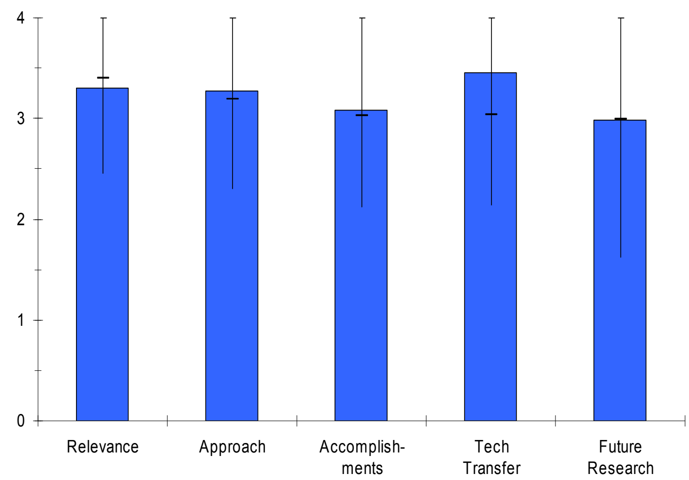
Weaknesses
- There is some concern that this project overlaps other efforts to identify suitable alloy combinations.
- There are some major issues associated with the oxidation and the embrittlement of the intermetallic material (B2) that have not been addressed.
- Reported membrane life is based on theoretical estimation and not actual experimentation.
- Hydrogen embrittlement is not only present in the membrane, but also the seals and other components, which have yet to be addressed.
- Need to address large scale application of methanol feed for hydrogen infrastructure
- Very little hydrogen transfer data.
- The project team has not addressed the durability (embrittlement) issue.

Specific recommendations and additions or deletions to the work scope

- The project team did not report thermal cycle results. Some thermal cycle studies are needed.
- Look into how the membrane materials can be applied for larger scale applications (500 - 3000 kg/day).
- Some focus on testing with H_2S is needed.

Project # PD-20: Sulfur-Iodine Thermochemical Cycle Laboratory-Scale Experiment
Paul Pickard; SNL/GA/CEA

Overall Project Score: 3.2 (7 Reviews Received)



Brief Summary of Project

The overall objective of this project is to determine the potential of the Sulfur-Iodine (S-I) cycle for Hydrogen production using nuclear energy and to: 1) explore the potential for high efficiency and technical maturity in sulfur cycles; 2) Evaluate and test process options, construct integrated lab scale experiment to demonstrate S–I cycle; 3) provide basis for cost projections and comparisons; and 4) support Nuclear Hydrogen technology selection decision (FY2011). The phase one objectives are to evaluate process options, establish baseline flowsheets, and conduct experiments on process options and materials. Phase two (Integrated Lab Scale Experiment – ILS) objectives are to: 1) develop and test the 3 major reaction sections for S-I; 2) assemble the 3 major reaction sections into an integrated, closed loop demonstration experiment; and 3) conduct S-I integrated lab scale experiments program.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

- It is recommended that long term durability studies on the materials be completed.
- The Sulfur-Iodine thermochemical cycle has been extensively evaluated and has promising hydrogen production efficiency. Demonstration of integrated loop process hardware compatible with next generation high temperature nuclear reactors will enable co-development.
- Efficient hydrogen production capability can be ready when the nuclear reactors are, and hopefully the rigid specification barriers in nuclear reactor system design will be chosen in a way not inadvertently exclusive of this hydrogen production pathway.
- Project supports Nuclear Hydrogen Initiative.
- Potential high efficiencies.
- The sulfur iodine process is well matched to the most likely design for the Next Generation Nuclear Plant project.
- Clearly makes H_2 which is DOE goal.
- Not clear technology could be available by 2017 to support DOE goals.
- Success in this area will support the development of a hydrogen economy.
- Is this the best opportunity for using nuclear energy for hydrogen production? Why was this cycle chosen? What about other cycles?
- This is the most advanced and most important project related to thermochemical water splitting using nuclear heat. One might argue that if this cycle isn't developed to high efficiency, then thermo chemical water splitting will be no longer considered for integration with the next generation nuclear reactor.

Question 2: Approach to performing the research and development

This project was rated **3.3** on its approach.

- Major issues have been identified.
- Would be good to see a critical path to achieve the 2011 goals.

- It seems that integrating 3300 bayonets is not a trivial problem. An advanced design for higher production rates may be required to minimize the quantity of bayonets.
- The trifurcation of process and hardware is a reasonable parsing of project capabilities, and promotes, hopefully, good collaboration among project partners.
- Scale of the process hardware is reasonably sized for proof of integration of the three main sections, while remaining small enough so that substantial changes in individual components could be affected at reasonable cost.
- Partners operate 3 independent reactor sections then combine for shake down in 07 closed loop 200 lph H_2.
- Good use of individual partners strengths at start of development.
- Project ties in with nuclear hydrogen initiative.
- Costs should be considered in evaluations of different approaches to addressing the major issues
- Three labs working together.
- Combining all lab work at GA seems to be a good approach.
- Need to assess risks with this process.
- Need to look at costs of complex metallurgy.
- Just because SI cycles are the most researched (as stated during presentation) doesn't mean that they are the most optimal.
- Good reactor design concept.
- PI should know how much hydrogen would be produced for the various scales being studied. Reveals a lack of understanding of the hydrogen markets that they're hoping to produce hydrogen for. Need a better systems understanding to appropriately design the production system they're working on.
- Extractive distillation is a good idea for this project. Shows that the project team is not sticking to only conventional systems.
- What about the concern about ceramics embrittlement?
- Excellent focus on overcoming technical barriers. Ties to INL to find alternative methods for concentrating HI solution are also good.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.1** based on accomplishments.

- Progress has been achieved, but seems that for the funding more progress should have been made.
- One of the objectives is to provide a basis for cost estimates. Nothing was reported on costs.
- The three principal process pieces have been designed, built, and apparently have met their specific targets for processing rates.
- The skid mounted sub-process assemblies are ready for integrated assembly. On target for integrated mode testing.
- H_2SO_4 decomposition corrosion issue addressed with SiC bayonet design allows high temp ceramic section with low temp process connections.
- No seals in reactor at temperature.
- Economic impact of additional step for phosphoric acid for HI should be reviewed.
- X and Y axes on the SO_2 production charts should be in the same units (ideally, moles SO_2/hr v. moles H_2SO_4/hr). Also, it is not clear whether "moles acid/hr" refers to moles of H2SO4 or moles/hr of solution at, for example 38 mole % H_2SO_4. Comparing L of SO_2 to moles of H_2SO_4 is not very user friendly.
- Experiments under way at 3 sites.
- Appears to be high-quality experimented work.
- Very good progress on planned research.
- Not sure that the costs presented in response to questions pass the laugh test.
- Excellent work on new reactor design, including easily-scaled reactor.
- Good progress has been made but the use of phosphoric acid in the HI concentration step adds a lot of complexity and risk to achieving acceptable efficiency. More emphasis should be placed in developing alternatives that have less complexity.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.5** for technology transfer and collaboration.

- There appears to be good coordination and well defined rolls for the team members.
- The project partners and scope were chosen in a way that should assure good excellent collaboration; we will see shortly if this worked!
- Integrated process testing at GA is a good way to assure that Next Generation HTGR's will be Hydrogen Production ready.
- Good mix of partners from national labs universities, industry and international.
- How will this project benefit from the lessons learned in the other high temperature integrated laboratory scale experiments?
- Collaboration / design of work among 3 sites.
- Not clear how much collaboration occurs outside of core group.
- Doing significant amount of process development without process collaborator to do significant cost analysis.
- Good project team.
- Excellent recognition that works elsewhere can help this project.
- The project shows excellent cooperation across institutions and has a definite pathway for commercialization.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- Team integration and testing work appear to be well planned.
- One of the stated goals is to provide basis for cost estimates. This is not clearly discussed.
- The investigators should define some Go/No go decisions for off ramps.
- PI reported \$2.79 H_2 per kg at 5 cents per kW power during Q&A but should include details of cost estimate in next years review.
- Experiments should evaluate the costs versus benefits of various approaches to resolving the primary issues. For example, to evaluate maximizing heat transfer to the catalyst versus longer residence time and improved catalyst surface area/support.
- Next step is to operate integrated skids.
- Good total-project plan.
- Should have a working prototype by the end of the process.
- Need a greater focus on analysis; how is research being defined?
- Future plans make sense and are well focused on problem solving and demonstration of the technology.

Strengths and weaknesses

Strengths
- There is a strong team that has clearly defined roles and appears to be working well together.
- Project partners' basic capabilities coupled with their shared leadership in developing next generation HTGR's.
- Selection of a solid thermochemical cycle with production efficiencies compatible with production quantities needed for the hydrogen economy.
- Process design, reaction kinetics, and material selections (for the HI and Bunsen sections at least) once proved can be utilized to make H_2 by other primary heat resources of sufficient temperature; principally solar thermal.
- SiC Bayonet reactor design eliminates seals.
- ILS appears to be designed for flexibility and incorporates the ability to run sections separately and exchange process equipment as needed.
- Well organized, good project team, good plan.
- Project strengths are the team and the significant investment in the technology that has been made over the last thirty years.

Weaknesses

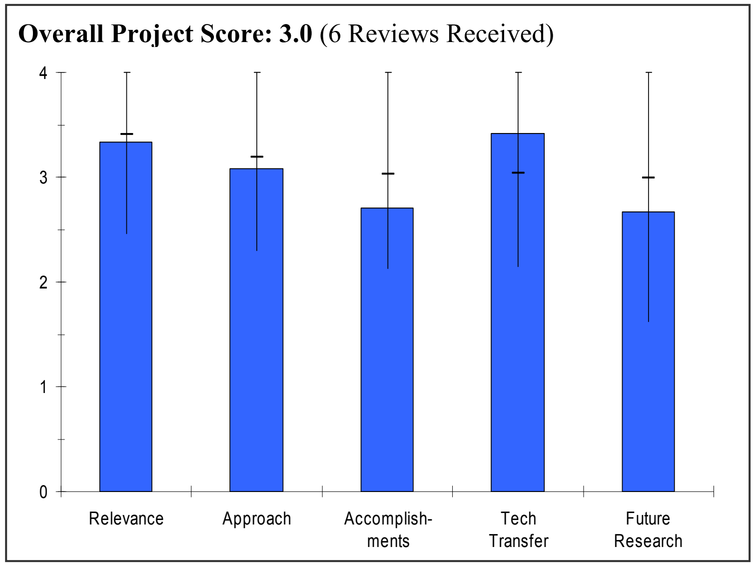
- There are substantial materials problems, such as the catalyst degradation, that will need to be overcome.
- Integration and control of 3300 bayonet heat exchangers/reactors may be very difficult.
- The exotic materials most likely required may be very expensive.
- Reaction kinetics, proper sizing of inter-process transport and reactant carryover are interface issues of concern as the three skids are integrated.
- Assuming good closed loop(s) process results are demonstrated, doubts about scale-up could still hinder further development opportunities.
- H2SO4 decomposition catalyst deactivation potential for short reactor life.
- Many of the process steps do not seem to be well enough developed as independent unit operations to support integration.
- Need more economic analysis. This is a very complicated process utilizing expensive metallurgy and it must be shown to be better than other alternatives.
- Need better analysis.
- The most obvious weakness is the complexity of the phosphoric acid extraction step.

Specific recommendations and additions or deletions to the work scope

- It is recommended to include in a later phase the design of an advanced reactor design to enlarge the reactor so that not as many bayonets will be required for control and integration.
- It is recommended that durability studies on the system be included in the next phase. It is unclear that these studies were planned.
- Continue to share information on achievements and challenges with the Solar Thermal Thermochemical project participants.
- Complete corrosion testing of mixed acids in HI section.
- Project is well focused and needs no additions or deletions.

Project # PD-21: Hybrid Sulfur Thermochemical Process Development
Bill Summers; SRS

Brief Summary of Project



The overall objective of this project is to develop the Hybrid Sulfur thermochemical cycle and demonstrate in an integrated laboratory scale experiment producing >100 lph of hydrogen. The objectives for fiscal year 2006 were to develop and test an SO2 depolarized electrolyzer (SDE) using polymer electrolyte membrane (PEM)-type cell design, including to: 1) characterize, analyze and select cell components; and 2) test single cell SDE electrolyzers at elevated temperature and pressure. The objectives for fiscal year 2007 are to: 1) develop improved electrolyzers; 2) demonstrate extended operation capability; 3) scale-up to larger size; 4) continue to identify and develop improved cell components; 5) conduct 100 hour longevity test on single cell SDE; and 6) design and build multi-cell SDE with 100 lph hydrogen capacity.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

- Focused on H_2 which is DOE goals.
- Technology is high capital / long term solution. Not clear can assist to meet 2015 DOE goals.
- Focus can only be on a large regional plant.
- This project would be more relevant to the future H_2 economy if it would focus on success of hybrid sulfur process. Inclusion of electrolyzer development and testing seems to be a diversion.
- Presentation should supply information on why the hybrid sulfur cycle was chosen over other options.
- DOE has appropriately chosen a project on the hybrid sulfur cycle.
- On the basis of the KISS (Keep It Simple, Stupid) philosophy, this project is critical to NHI for H_2 production that is cost-effective, provided that SRNL can solve the SO_2 cross-over.
- The combination of thermo chemical and electrochemical processes for producing hydrogen detracts somewhat from the overall goal of producing both hydrogen and electricity using high temperature nuclear heat. Electricity at 7 cents per kW is more valuable than hydrogen at $3/kg.
- The project goals are critical to the Hydrogen Initiative and fully support DOE RD&D objectives for thermochemical process development for hydrogen production.

Question 2: Approach to performing the research and development

This project was rated **3.1** on its approach.

- Focus on electrolyzers is appropriate for this project.
- Approach is reasonable.
- For cost this appears to be a simpler / higher probability of success than other nuclear programs.
- Input of electricity is a drawback.
- Oxygen byproduct should not be shown as a bonus. Unless the nuclear power plant is next door to a gasifier, there's probably not an economical market for it.
- Need to address corrosion.
- Emphasis is on developing a PEM-type cell design and improving membrane performance, which are key.

- Determination of critical thermo physical properties is critical to obtain a good model.
- There are significant challenges with respect to the choice of anode materials, the development of new membranes that do not pass sulfur dioxide and the operation of the electrochemical cell at high sulfuric acid concentrations. Although all four of these points were raised and discussed by the investigator, no clear alternatives were offered for overcoming these problems. For example, the investigators have limited themselves to investigating only those membrane electrolytes that are commercially available. Fuel cell developers, on the other hand, are putting significant effort into developing better membranes for their applications which are technically less demanding than those of the proposed electrolysis cell.
- The project subtasks are well-focused on specific technical barriers.
- The project subtasks are well-balanced with respect to different technical barriers.
- The approach builds upon well-established technology, ensuring compact design and attractive unit costs.
- The contributions and responsibilities of collaborators and partners were clearly described.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.7** based on accomplishments.

- Cells need to be tested at higher acid concentrations and pressure and for longer durations.
- Good thought process of why technology might work and why this would be economically attractive.
- 100 hour test is not adequate progress given that this project started in 2004.
- Using specialized materials of construction do not help this project address corrosion concerns.
- The patent for this process was issued in 1975; need to show what progress in thought, if not R&D, has been made since then.
- What about cost analysis? Costs given verbally during Q&A are completely unbelievable.
- Good progress, but it appears that a breakthrough is necessary for the membrane work. Very difficult problem.
- A more quantitative discussion of the SO_2 carryover would have been useful for an assessment of the difficulty of this challenge.
- This project has succeeded in identifying several show stoppers. Among them are high cell voltage and sulfur dioxide crossover from anode to cathode. The investigators are only beginning to understand the magnitude of the problems with this system and have not yet charted a pathway to overcoming these barriers.
- The selection or derivation of specific milestones and performance indicators was well-described, with excellent progress towards specific performance parameters.
- The progress has been especially strong for the single cell testing, which reached a key milestone ahead of schedule.
- The progress is very well-documented with respect to specific components.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.4** for technology transfer and collaboration.

- Leveraging of existing PEM research is beneficial.
- The project partners appear to be working closely with each other to develop and improve the electrolyzers
- Good set of collaborators.
- Why Giner? Suggest broadening to other electrolyzer manufacturers.
- How does this project connect with SNL/GA/CEA project?
- How is Westinghouse involved in the project?
- The mix of participants is sufficient to bring this technology from the laboratory to commercialization.
- There is strong partnership and integration with other institutions and industrial enterprises.
- The characterization of experimental membranes is derived from commercially-available sources, ensuring a focus on the partners' respective expertise.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.7** for proposed future work.

- Costs and potential value of byproducts should be evaluated (excess heat and oxygen).
- It is not clear that a complete integrated laboratory scale experiment, including the acid thermal decomposition step is necessary given that this step is being extensively studied for the sulfur iodine process.
- More extensive research seems to be needed on the long term performance of the cells under operating conditions and for catalysts.
- A specification for sulfur deposition to work toward should be developed.
- Does not appear to include economic analysis.
- Stating that improved membrane will be researched, "...with industry partners" is inadequate. Is there a company lined up or is the presenting team hoping to find someone to work with?
- Longer duration tests should be planned; 100 hours is not adequate.
- Not enough detail presented on FY08 plans. What about plans beyond that? Project is supposed to end in 2010; how do you know that without a plan?
- All of the future work described is necessary. The emphasis on improved cell membrane is appropriate.
- Future research should include membrane development and work with non noble metal catalysts.
- The future research continues to build towards meeting established milestones, and overall schedule performance is strong.

Strengths and weaknesses

Strengths
- Close collaboration of partners and use of prior PEM research
- Interesting cycle being studied.
- Good membrane work, although there is a question about whether electrolyzer development should be included in this project. It may dilute the effort.
- The project's primary strength is the past work that defined many of the operating conditions and a preliminary flowsheet to build on.
- Another strength is the simplicity of the cycle and involves only S, H_2, and O_2.
- Project strengths are the experience of the teams and the long history of work on this technology.
- The investigators demonstrate clear experimental design of each subtask, and have made significant progress in the project.

Weaknesses
- The project PI did not seem to be aware of newer research in electrolyzer catalysts.
- Needs more economic analysis – is nuclear Rx free – is energy (electricity and heat) free?
- Needs to look at materials needed and costs.
- Electrolyzer research dilutes effort on hybrid sulfur cycle.
- Insufficient depth in project team.
- No total project plan.
- No mention of past work.
- Westinghouse reported an integrated lab demo in 1976, where, I think, 100 L of H_2 / h was produced. Has the old technology been fully examined? SO_2 carryover and S deposition were problems in the 1970s and there was mention that progress was made in mitigating the SO_2 carryover in the 1970s.
- There seems to be a desire to focus on building demonstration cells rather than focusing on understanding to chemistry and electrochemistry. Perhaps this is the result of the program focus on demonstrating liters per hour rather than efficiency and durability.
- Contingencies are not described, and it is not clear how the investigators will actually use "innovative design approaches" to improve upon commercially-available membranes.

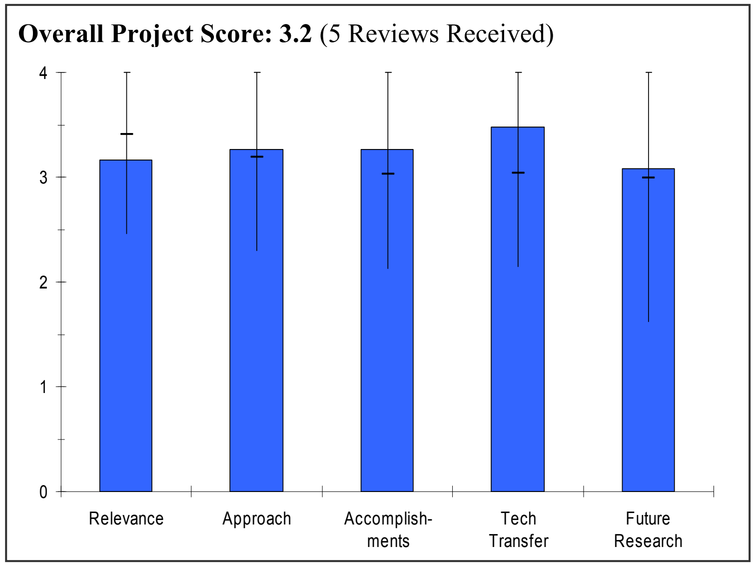
Specific recommendations and additions or deletions to the work scope

- Delete full HyS process integrated laboratory scale test; instead develop a joint integrated test with the sulfur iodine process.
- Needs to determine what are research goals to meet DOE targets.
- Project seems to be focused on building and testing equipment – needs to focus on economic viability.

- Expand partners.
- Transfer electrolyzer research to another project.
- Add work on developing a fundamental understanding of the electrochemistry and the membrane. Also, producing high concentrations of sulfuric acid may be incompatible with a membrane cell that depends on high levels of hydration for good ionic conductivity. The specifications for the electrochemical cell are too severe. Concentrate the sulfuric acid elsewhere in the system.

Project # PD-22: Laboratory-Scale High-Temperature Electrolysis System
Steve Herring; INL/ANL/Ceramatec

Brief Summary of Project



The technical objectives of this project are to: 1) Develop and demonstrate energy-efficient, high temperature solid oxide electrolysis cells (SOECs) and stacks for hydrogen production from steam; 2) demonstrate technology at progressively larger scales; 3) perform flowsheet analyses of systems-level high-temperature electrolysis (HTE) processes to support planned scale-up to Integrated Laboratory-scale, Pilot-scale and Engineering Demonstration-scale experiments; 4) develop detailed computational fluid dynamics (CFD) models of operating SOECs; validate with experiment data; and 5) investigate alternate cell materials (e.g. alternate electrode and/or interconnect materials) alternate cell configurations (e.g. porous-metal substrates, tubular cells, porous electrodes) and applications of inorganic membranes.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.2** for its relevance to DOE objectives.

- High temperature electrolysis is definitely within the Hydrogen Initiative.
- The project supports the NHI and is in-line with the goals at the NHI.
- The development of a high temperature water electrolyzer that operates at high efficiency is certainly relevant to the DOE goals. However, the tie to high temperature nuclear reactors is not clear, since the only thing the nuke supplies is electricity. This could just as easily be tied to renewable energy sources.
- This project is consistent with the DOE program on the Nuclear Hydrogen Initiative.
- There is a concern, however, about co-locating a major hydrogen facility in close proximity to a major nuclear facility.
- There was also a comment during the Q&A in this session that such a hydrogen facility would only be for a captive large-scale user, such as a tar sands upgrading facility. This seems to be inconsistent with the EERE hydrogen production program in general, and the needed quality of the hydrogen product may be quite different for automotive use versus refinery use.

Question 2: Approach to performing the research and development

This project was rated **3.3** on its approach.

- Good plans for FY07 and 08, but it would be nice to see a high level plan to achieve the engineering demo in 2015.
- Leveraging off of DOE's SECA program is a good approach to improving the SOEC.
- Did the presenter consider other sources for SOFC's?
- The multi-center complex project is well-organized.
- The approach of progression from button – we test through laboratory and pilot scale to an engineering demonstration facility is well-designed.
- The project builds on research from the SECA and other programs.
- Testing to date seems to have identified the major issues and work has been done to address them.

- The approach being taken appears to concentrate on building demonstration cells before a complete understanding of the technology has been developed. The approach is to take the technology developed for solid oxide fuel cells and run it backwards. It is obvious from the presentation made by the investigator that this approach has problems.
- The approach uses a good combination of progressive experimental development (from a button cell to a 25-cell stack, to 60-cell stacks, to 4-stack modules in the integrated laboratory-scale experiment) and process and component performance modeling and analysis (flow sheet analyses, CFD analyses of cells, stacks, and modules).
- It was not clear if the larger systems, such as 200-kW pilot plant and the 1-MW engineering demonstration, would use the same size cells/stacks/submodules as in the current work or if these larger systems would require significant scale-up in cell size and/or number of cells per stack. Such scale up is not likely to be a simple extrapolation of current fabrication, assembly, and control processes and systems.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.3** based on accomplishments.

- The analysis work and design work are accomplished.
- How was progress from SECA work leveraged into the SOEC?
- The durability tests appeared to provide useful information.
- A chart that compares their progress with the DOE goals and other technologies would be useful.
- Delamination at the electrodes too been significantly reduced.
- Design of the integrated lab scale experiment has been completed and fabrication --> well underway.
- Decreasing electrolyzer cost is being addressed through development of longer format cells and evolution of other geometrics.
- Stack life-time is a concern.
- Lessons learned from the work done to address the delamination and cracking problems should be presented.
- Despite the problems of material degradation and delamination, significant progress has been made in developing and testing 22 and 25 cell stacks.
- A major accomplishment has been the 2000-h test of the 2 x 60-cell stacks, yielding from 0.6 to 1.2 normal cubic meters of hydrogen per hour (test run stopped due to shorting of the current leads to the manifold).
- Another major accomplishment has been the post-test evaluation of cells from the earlier 25-cell stack. Based on some of the answers during Q&A, the results of those analyses are being used to help improve the materials and fabrication processes for new cell and stack builds.
- The ILS development appears to be proceeding well with development of the piping and instrumentation diagram, design of steam generator/superheater, and fabrication and delivery of ILS modules (electrolyzer stacks).

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.5** for technology transfer and collaboration.

- Good participation by national laboratories, more industry participation would be useful.
- There were an impressive number of publications.
- There appeared to be relatively open discussion of the fuel cell performance and how to improve it.
- This project is a well coordinated effort of multiple centers and an industrial partner.
- Better integration with the solid oxide fuel cell research program would benefit this project.
- The team working on this project is well qualified to bring this technology to market.
- The project team has members from other national laboratories and industry.
- Although "clear path to commercialization" was identified as an FY-07 THE issue/concern, there was no discussion of how that would be attempted, particularly since no nuclear industry participant has been identified.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.1** for proposed future work.

- Plan with built in Go/No go decision points and off ramps is necessary.
- There has been sufficient development to be able to perform a cost analysis, which should be included.
- The project plan for future years is well laid-out.
- The project is evaluating alternate SOEC geometries at the bench scale while moving forward with testing of the 240-cell SOEC in the Integrated Laboratory System.
- Further work is needed to address performance degradation.
- The plan should include more fundamental work studying new materials and electrochemistry. Questions were raised at the presentation that indicated that even the cell geometry may be in question with the suggestion that the team is considering switching to tubular cell geometry. This needs to be sorted out quickly.
- The activities listed for future work are heavy on testing but light on the development of improved materials and processes. Perhaps the presentation did not touch on that, but the program plan includes it?
- Based on the discussion during Q&A, this project depends heavily on the developments and successes in the SECA (and other similar) program. Because of the reversed polarization and different water contents between SOEC and SOFC operating conditions, more emphasis on electrode and electrolyte materials for the SOEC application, particularly at lower temperatures, is likely to be more fruitful.

Strengths and weaknesses

Strengths
- The project has access to much of the technology being developed for SOFC fuel cells.
- The team has an impressive amount of publications.
- There was good progress made, especially performing a 2000+ hr test.
- The project is well-organized.
- The project builds on previous work.
- Good technical progress has been made.
- The project makes good use of previously developed information.
- This is an excellent team. They have at their disposal all the tools needed to succeed.
- The project includes a good mix of experimental, diagnostic, and analytical components (among the best such mix over the range of projects discussed in this session).
- The progression to successively larger test cells, stacks, and modules is commendable.

Weaknesses
- The long term goal was to show commercial viability, but there was not cost analysis.
- The stack lifetime was relatively short and there was no discussion on how to improve its life.
- The current status and development hurdle of the ORNL membrane was not adequately discussed.
- The impact of short stock life-time in system economics was not presented.
- Loss of performance has not been fully addressed.
- The project is attempting to adapt existing solid oxide fuel cell technology to operate outside the envelope for which it was designed.
- Considerable degradation has been observed in 25-cell and 60-cell stacks. It is not clear that the results of post-test analyses (completed at the end of November 2006) could be used effectively in the build of the ILS module (delivered in the second half of March 2007).
- Plots of the 25-cell and 60-cell stacks' performance over time would have been helpful. A technical discussion of the trend seen as well as a discussion of any diagnostics conducted during the long-term tests would have been very informative.

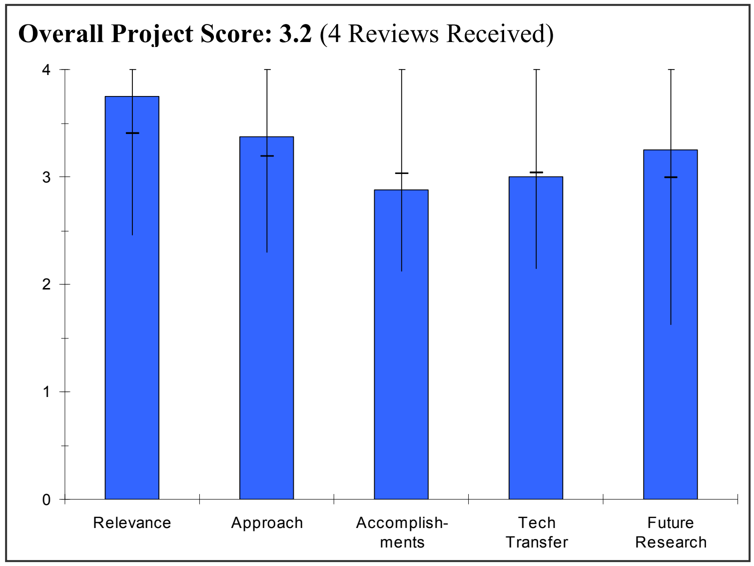
Specific recommendations and additions or deletions to the work scope

- Durability testing should be included
- Additional industrial partners would be useful; the project may want to consider other SOE vendors.
- A critical path, with risk mitigation and Go/No-Go milestones, to achieving the ambitious goals of 1MW demo in 2015 was not clear. This should be developed.
- It is recommended that a research university with significant experience in materials and solid oxide fuel cells be brought onto the team to investigate the fundamental materials science.

Project # PD-23: Nuclear Reactor/Hydrogen Process Interface
Steve Sherman; INL

Brief Summary of Project

The overall objectives of this project are to: 1) guide the development of technologies to enable the connection of a Very High Temperature [nuclear] Reactor (VHTR) to a high-temperature hydrogen plant; 2) resolve technical issues and challenges offered by the DOE Nuclear Hydrogen Initiative (NHI) and Next Generation Nuclear Plant (NGNP) Project in regard to nuclear connection design, construction, operation, safety, economics, and nuclear plant licensing; and 3) work closely with NHI Thermochemical and High-Temperature Electrolysis areas to define and test components and systems.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.8** for its relevance to DOE objectives.

- The purpose of the components database is not clear.
- It is not clear how this project will address technical issues having to do with economics as no costs or cost comparisons between alternatives have been presented.
- Required technology to provide for advanced high temperature reactor co-production of hydrogen and electricity.
- Research may also be applicable for solar thermal hydrogen production technologies.
- Linking the H_2 production plant with the reactor is critical.
- Emphasis on materials and heat exchange designs is well though out.
- This project is very relevant to the development of hybrid nuclear hydrogen systems. It addresses the bridge between the nuclear plant and the hydrogen generator. It is essential that this project identify and validate cost-effective materials compatible with both systems.

Question 2: Approach to performing the research and development

This project was rated **3.4** on its approach.

- This project should provide cost/benefit analyses for the various approaches to overcoming the barriers.
- Appears to take a comprehensive approach to the R&D effort.
- Good configuration management, ensuring that all changes made in materials, components, safety features, etc. are re-checked for their impacts on the other critical design parameters.
- Logical narrowing of R&D foci to the critical parameters.
- Approach is focused on technical barriers and, if implemented, will lend to an integrated nuclear plant and a hydrogen plant.
- The approach is well defined and focused on solving the problems and overcoming the barriers to interfacing the high temperature nuclear reactor with the thermo chemical water splitting system.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.9** based on accomplishments.

- The presentation was not specific enough regarding accomplishments.
- No cost or performance information was presented for the heat transfer loop as requested by previous reviewers.
- Appear to be narrowing in on many of the viable materials and design options.
- Integrated system modeling that interfaces with the reactor side modeling.
- Specific materials and components development plan.
- Costs are high for the level of accomplishments: GA work on materials for HIx – Section 3 work is listed as an accomplishment both here in PDP 31.
- INL accomplishments are not explicitly defined and matching funds spent with INL accomplishments was impossible for this reviews.
- Good progress is being made although the project could be moving faster.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- The presentation did not clearly address how this project will facilitate transfer of information to and between the various high temperature demonstration projects.
- Strong collaborations with academia, private industry, national labs and foreign entities with common interests.
- Collaborators are many – 16 partners are listed. Coordination of this many projects is difficult to achieve with one person as lead with this many collaborators.
- This project has a team well positioned to commercialize the technology.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.3** for proposed future work.

- "Continued research" is proposed, but there are no clear criteria for success or prioritization of research needs.
- Well developed schedule for future work that was developed in collaboration with the NGNP project to ensure that the time when one project is waiting on the other for design input is minimized.
- Cannot tell if there are any optional paths built in, but the optional paths appear to be identified at least.
- Coordination with other laboratories appears weak. For example, INL proposes to initiate lab-scale testing of prototype heat exchanges, but this work is ongoing elsewhere. Future research for INL should be listed separately. Optional paths are being considered.
- The future plans are well focused and have a good probability of success.

Strengths and weaknesses

Strengths
- Well organized and coordinated with nuclear plant project, taking full advantage of a wide spectrum of resources and expertise.
- Work is well organized and critical needs are being addressed.
- The greatest project strength is the experience of the team.

Weaknesses
- None observed.
- Project will continue to become more and more complex as time line to full implementation comes closer. Need better coordination effort.
- The greatest weakness is not with this project but with the barriers that still must be overcome in developing the thermo chemical water splitting cycle that is to be interfaced with the nuclear reactor.

Specific recommendations and additions or deletions to the work scope

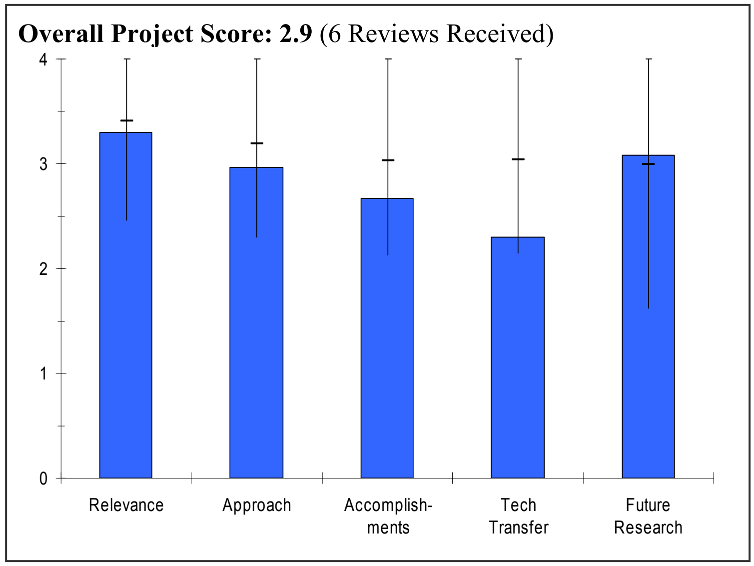
- None

This project is well focused. No additions or deletions are recommended.

Project # PDP-01: A Novel Slurry-Based Biomass Aqueous Phase Reforming Process
Ying She; UTRC

Brief Summary of Project

The objectives of the project are to: 1) illustrate, through initial feasibility analysis on a 2,000 ton/day (dry) biomass plant design, that there is a viable techno-economical path towards DOE's 2012 efficiency target (43% lower heating value (LHV)); 2) assess the requirements for meeting DOE's 2012 cost target ($1.60/kg H_2); and 3) demonstrate, through preliminary results, that an acid-tolerant, model sugar or sugar alcohol solution reforming catalyst has been synthesized. Future work will include hydrolysis work, catalysis discovery and testing, micro-scale continuous operation of membrane reformer with batch hydrolysis, and a final economic and energy analysis.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

- Although the hydrolysis approach may be well suited to certain feedstocks, it is unclear that it will be cost-competitive with more conventional gasification approaches over a wider range of feedstocks. Overall hydrogen production will be lower since lignin component is used for process energy only.
- Difficult to see how this process, with the added step of pretreatment, can compete with a gasification process.
- If process is incorporated with a fermentation process, the pretreatment might make more sense, but taking a dry (or relatively dry) feedstock and adding a dilute acid for the purpose of partially decomposing the biomass prior to a catalytic process that may or may not tolerate the acid and/or the water, seems unlikely to be cost-competitive.
- Analysis shows some promise, but a number of favorable assumptions have to be made about the catalyst and the process.
- Addresses DOE Program goal of low cost hydrogen production from renewable resources.
- Addresses barriers of reducing capital cost and improving efficiency.
- Biomass key element of DOE program.
- Highly rewarding if successful in converting biomass to hydrogen. The liquid phase reformability is key.
- Project supports MYPP.
- Project represents low greenhouse gas emissions process.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- Process flow and economics assumes high energy recovery from lignin combustion. The team needs to better address the issues that will be associated with the grade of lignin that will be coming out of this acid-treatment approach. High amounts of inorganics (alkali, etc) are likely and will greatly lower fuel value of the lignin.
- Good use of experimental design.
- It is unclear how much benchmarking of the current state of biomass hydrolysis has been performed.

- The analysis was thorough, although it is not completely clear why they performed sets of analyses where only a single parameter was varied, in addition to analyses where multiple parameters were varied (second set more useful in mapping out the experimental space).
- Overall approach involving biomass hydrolysis and aqueous phase reforming is based on known chemistry and appears sound.
- Suggest adding an early step in the program to test tolerance of aqueous phase reforming catalysts to heteroatoms expected in the hydrolysate e.g. HCl, SO_x or H_2S, NH_3 plus alkali metals.
- Should consider a "plan b" for hydrogen purification as no cost effective, robust membrane systems for removing hydrogen from this specific gas mix have been identified. Not at all clear that the proposed Pd membrane is affordable or stable to the various heteroatoms expected in the reformate (HCl, SO_x, NH_3, etc).
- Staged approach with upfront economic analysis is sound.
- Should do tornado diagram analysis on key conclusions looking at impacts of economic basis.
- Liquid phase reforming is attractive because of the lower temperatures.
- Kinetics are slow, byproducts are likely to be numerous.
- A Pd-based membrane does not appear attractive because of cost, contamination, and flux limitations.
- Limited early H_2 membrane testing.
- Limited catalyst life testing planned.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.7** based on accomplishments.

- Recommend performing sensitivity analysis around sulfur emissions and lignin combustion value.
- Progress is reasonable given low funding levels.
- Interesting analysis results.
- Good approach to catalyst development/discovery.
- Project appears to have just gotten underway, starting with a process modeling exercise. No experimental work done to date, and that is understandable
- The process and economic modeling predicts hydrogen costs that appear to be unbelievably low. Capital cost appears very low for a process of this complexity and requiring a Pd membrane module for H_2 cleanup. Feedstock cost also seems low. No accounting for disposal of by-product ash. Suggest researchers carry out a real cold eyes review with experienced industry veterans and DOE staff to validate these expectations of low cost.
- Little money so far so no expectations.
- Funding delays have limited work.
- System simulation and analysis has been conducted.
- Project at 2 year point (about 60% of project life), but only 10% complete – DOE funding to date about 20%.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.3** for technology transfer and collaboration.

- Funding limitations have limited tech transfer/collaborations.
- Industry-led project.
- North Dakota Energy Center listed as a partner...not clear how they are contributing or plan to contribute.
- Partnership of UTC and UND. Should set up "association" with similar biomass projects.
- Don't have the answer but UTC and the University of North Dakota seems light on partnerships.
- Role of UND is not clear.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.1** for proposed future work.

- Need to include lignin combustion characterization and sulfur recovery in future plans to validate efficiencies and economic assumptions.
- Effective and sulfur-tolerant catalyst discovery is critical to continued effort.
- Experimental plan is sound, but should address the comments made above regarding impact of heteroatoms in feedstock on performance of hydrolysis reaction, reforming, and separations.
- Approach is fine.
- Demonstration of the performance of an acid tolerant sugar reforming catalyst is very important.

Strengths and weaknesses

Strengths
- Strong capabilities in process modeling, economic analysis and catalyst development.
- Good process engineers, with systems analysis support.
- Interesting approach for catalyst discovery.
- Clear "gated" approach.
- Promises hydrogen from renewable biomass.
- Liquid phase reforming will be carried out at lower temperatures.

Weaknesses
- As mentioned, process economics and system efficiencies rely heavily on assumptions regarding lignin combustion. Technical challenges around this have not been adequately addressed.
- Pretreatment adds a lot of complication to the process that may not add much value unless byproducts are produced.
- Only 2 collaborators. Neither has industrial experience in field of study.
- Reformability of the biomass slurry.
- Tolerance of the Pd-membrane to the byproducts.
- The reaction is slow, hydrogen release is slow. Hydrogen concentration in the gas phase will be low, only part of which will be transported across the membrane. What is the expected final hydrogen yield (kg H_2 per kg of biomass slurry)?
- Will this process require subsequent methane reforming?

Specific recommendations and additions or deletions to the work scope

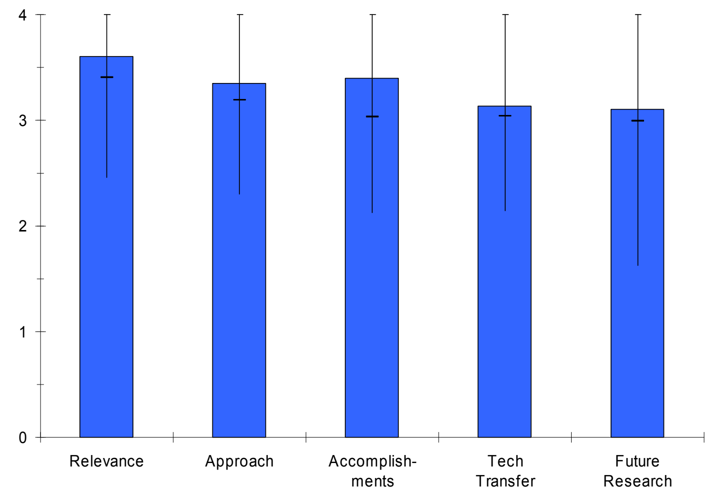
- Investigate potential interactions with cellulosic ethanol processes.
- Establish the liquid phase reformability before moving on to hydrogen separation and recovery.

Project # PDP-02: Hydrogen from Water in a Novel Recombinant Oxygen-Tolerant Cyanobacteria System
Qing Xu; Venter Institute

Brief Summary of Project

The overall goal of this project is to produce a cyanobacterial recombinant to produce H_2 continuously. The objective is to develop an O_2-tolerant cyanobacterial system for continuous light-driven H_2 production from water. Cyanobacteria have the ability to split water photolytically into O_2 and H_2, but their hydrogenases are highly O_2-sensitive. In contrast, certain bacteria have O_2-tolerant H_2-evolving hydrogenases, but they can not use water as the electron donor. The approach of the project is to transfer O_2-tolerant hydrogenases into cyanobacteria by 1) identifying novel O_2-tolerant hydrogenases from the Venter Institute's sampling in international waters and transferring them into cyanobacteria, and 2) transferring known O_2-tolerant hydrogenases into cyanobacteria.

Overall Project Score: 3.4 (6 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.6** for its relevance to DOE objectives.

- Effort is focused on fundamental issues related to long-term renewable hydrogen production.
- Multiple methods for producing hydrogen will be needed, and this project supports the objective of having a diverse portfolio of technologies.
- The project has a high potential for supporting the hydrogen fuel initiative.
- The project provides a unique and desirable niche with the HFI.
- The project could make significant contributions to the stated barrier of the continuity of hydrogen photo production.
- The direct advancement to overcome or broaching the relevant barrier was not addressed in the report.
- The combination of bioprospecting and metabolic engineering is very interesting and has significant potential.
- The project goals are critical to the Hydrogen Initiative and fully support DOE RD&D objectives for hydrogen production.
- Ties directly to the program goal to "Develop advanced renewable photoelectrochemical and biological hydrogen generation technologies".
- Project is high-risk, long-term R&D which provides balance for the program's shorter term hydrogen production efforts.
- Project supports MYPP long-term biological RD&D.

Question 2: Approach to performing the research and development

This project was rated **3.4** on its approach.

- Looking to nature to identify good candidates, and then transferring genes to an appropriate host.
- High-risk, long-term research.
- The approach has a high risk of technical failure.
- Process/culture options for removal of oxygen should be explored.
- Information regarding the robustness of this organism, normal growth rate, normal culture needs (e.g., required rate of sparging with air), acceptable temperature range, etc. in absolute terms and as compared to other bacteria

was not presented. This information will be critical to determining whether the "view is worth the climb" for this project. A fast growing, non-fussy, "low-maintenance", CO_2 eating bacteria that can be dried out and used for biomass, and also produces a little hydrogen while it's growing would probably be much more valuable than a slow-growing, "high-maintenance" organism that produces a little more hydrogen.
- The approach is appropriate and the group is making interesting and significant progress.
- The limited number of hydrogenases identified is somewhat of a surprise and the investigators could consider mechanisms to probe deeper into the diversity of the environments further exploiting the available vast metagenomic data.
- The potential for controlled expression of hydrogenases in cyanobacteria is a very exciting element of the project.
- The project subtasks are well-focused on specific technical barriers.
- The project subtasks are well-balanced with respect to different technical barriers.
- The project subtasks are clearly designed to integrate with other research supported by the DOE Hydrogen Program.
- I would like to see a vision presented of how such a system would work in practice if a suitable organism could be engineered, and what the water and land (or other) resource requirements would be, at least in a general way. There is no discussion of what the barriers might be beyond the development of the organism itself.
- Straightforward strategy to transferring hydrogenase enzymes with desired oxygen tolerance to organisms of interest.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.4** based on accomplishments.

- Good level of accomplishment, especially considering the lack of funding.
- A great deal of work has been accomplished. A great deal more is needed.
- The group is making significant progress in the two major thrusts of the project: a) the identification of new stable hydrogenases and b) the heterologous expression of hydrogenases identified in nature.
- Probing the vastly and rapidly accumulating metagenomics data for potential contributions to the hydrogen fuel initiative is very important and merits continued support.
- The selection or derivation of specific milestones and performance indicators was not evident; however, the progress towards specific performance parameters has been excellent. What specific metrics will be devised to determine desired thresholds of oxygen tolerance in combination with volumetric productivity of hydrogen evolution?
- In evaluating this project as a research endeavor, the progress has been outstanding. There have been a few significant publications resulting from this funding, demonstrating excellent progress for such a recently-initiated effort.
- The identification of candidate oxygen-tolerant hydrogenases from a bioinformatics survey of the Global Ocean Sampling project was a significant technical accomplishment. The identification of novel hydrogenases is a good beginning to guide evolution of the Thiocapsa hydrogenase to even higher oxygen tolerance and activity.
- The progress in expression of these novel hydrogenases in Thiocapsa was good, although it was unclear whether activity had been demonstrated. If so, how did that activity compare to the endogenous hydrogenase in this organism?
- The heterologous expression of the Thiocapsa oxygen-tolerant hydrogenase and corresponding maturation proteins in Synechococcus was a good technical accomplishment.
- The heterologous expression of the Rubrivivax oxygen-tolerant hydrogenase and corresponding maturation proteins in Synechocystis was a good technical accomplishment, with demonstration of hydrogenase activity. It was unclear how the level of activity was benchmarked, and what was the eventual target.
- The progress has been all the more remarkable given the minimal level of FY06 funding—with most funding contributed by the Venter Institute.
- Need to keep in mind the DOE's ultimate goal here, which is "By 2018, verify the feasibility of these technologies to be competitive in the long term". So, as project progresses, some attention to system engineering and costs will be needed to make go/no-go decisions on this pathway.
- Progress seems to be good, particularly given lack of DOE funding in 2006.
- Good process despite lack of funding.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.1** for technology transfer and collaboration.

- Good collaboration with NREL.
- DOE is getting a lot for their money on this project.
- The group has an ongoing cooperation with NREL and has the potential for broader collaborations as the work progresses, especially at academic institutions.
- Most of the research is not developed to the point where opportunities for technology transfer are apparent.
- There will obviously be opportunities for intellectual property development and tech transfer; however, the mechanism may be complex due to the individual MTAs developed for the countries with jurisdiction over the sites employed in the GOS.
- The investigators demonstrate good coordination and collaborations with university researchers.
- The investigators demonstrate good coordination and collaborations with international researchers.
- It is unclear what, if any, coordination or collaboration has been done to explore other, similar, work in this field.
- Have any papers been published and presented at technical conferences?

Question 5: Approach to and relevance of proposed future research

This project was rated **3.1** for proposed future work.

- Plan builds on progress.
- May need to have more definitive strategy for discontinuation of work with specific organisms.
- The project is progressing at a steady pace, and future plans continue to support the long process of developing a viable hydrogen producing organism.
- The proposed plan is appropriate for the level of support dedicated to the project.
- A more clear description of the mechanism by which active expression in the cyanobacterial host might be achieved and potential contingencies in the experimental design would strengthen this component of the work.
- A potential avenue for increasing the scope of the work is to implement a mechanism to probe whether additional hydrogenases exist within the metagenomic sequence data collected from these environments.
- The investigators clearly present a plan to build upon their discovery-driven success for designing an oxygen-tolerant hydrogenase, through additional characterization of the novel hydrogenases identified from the GOS.
- The plan to improve Rubrivivax hydrogen production through refinement of corresponding accessory genes and heterologous expression in Synechocystis is a logical next step after the proof of principle in E. coli.
- Again, project should address potential systems-level barriers – the ultimate goal is cost-effective production of large amounts of hydrogen, not the design of a new microorganism.

Strengths and weaknesses

Strengths
- Dedicated participants.
- Good understanding of the concept.
- Venter Institute and NREL collaboration appears to be very strong and beneficial to DOE.
- The project represents a unique and attractive niche in the program.
- Although perhaps high risk, the project has the potential to offer something completely new.
- The combination of bioprospecting and expression directed toward metabolic engineering has exciting potential outcomes and is an outstanding strength.
- The expertise of the group approaching the project is excellent for the proposed work.
- The investigators demonstrate clear experimental design of each subtask, and have made significant progress in all initial phases of the project.
- The tenacity of the investigators to obtain alternative funding and collaborators is to be commended.
- The team is expert in the study of hydrogenases, and the combination of a strong bioinformatics/genetics effort with a focused biochemical approach is excellent.

- The knowledge of these investigators for the microbial and algal systems under study is well-focused towards the project goals.

Weaknesses

- Difficult problem (high-risk research).
- Alternative methods for overcoming oxygen intolerance (such as the removal of oxygen) should be explored.
- There is limited attention to potential outcomes and contingencies in the cyanobacterial expression component.
- It is unclear how the results from the heterologous expression studies will be synergized--how will information obtained from the characterization of novel hydrogenases be used to improve the Rubrivivax studies? Are these all to be done in parallel, at separate labs – essentially two unrelated projects under a single umbrella? There should be a clearer definition of checkpoints and cross-talk for these experiments.
- The investigators have not clearly articulated what the targets or milestones are—are they seeking for a specific level of hydrogen production for a specific oxygen-tolerance? Have they thought about theoretical limits for these enzymes (when will they know they have sampled enough ocean samples to know there are no additional hydrogenases resembling the Thiocapsa proteins)?
- The proposed experiments are all focused upon comparisons and refinements of known hydrogenases. How will the investigators recognize novel forms of hydrogenases, which may possess the desired production and oxygen-tolerance targets but not resemble canonical hydrogenases? What if these hydrogenase activities require multiple subunits, or accessory factors that do not resemble those known to date?

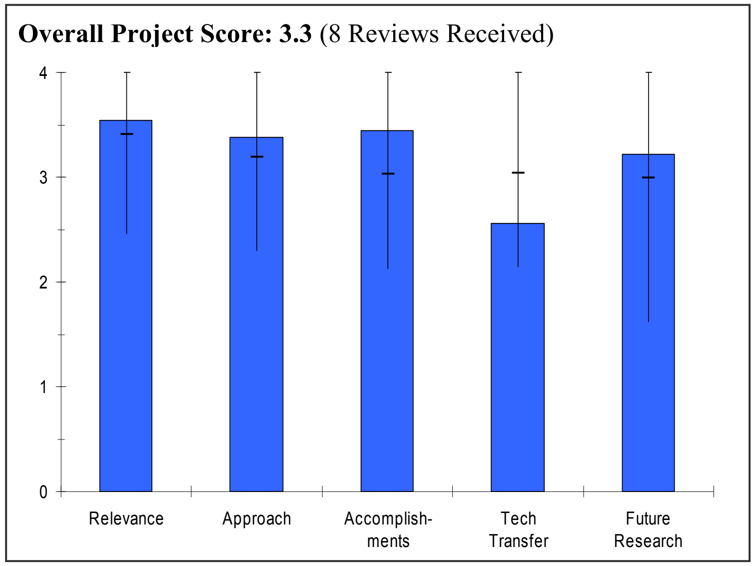
Specific recommendations and additions or deletions to the work scope

- Probing for additional hydrogenase (increased diversity) within the existing metagenomic data.

Project # PDP-06: Investigation of Bio-ethanol Steam Reforming over Cobalt Based Catalysts
Umit Ozkan; Ohio State U

Brief Summary of Project

The overall objective of this project is to acquire a fundamental understanding of the reaction networks and active sites in bio-ethanol steam reforming over Co-based catalysts that would lead to 1) development of a precious metal-free catalytic system which would enable low operation temperature (350-550°C), high ethanol conversion, high selectivity and yield of hydrogen, and minimal byproducts such as acetaldehyde, methane, ethylene, and acetone; 2) understanding of the catalyst deactivation and regeneration mechanisms; and 3) low cost for commercialization.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

- Development of a precious-metal free, low temp. Ethanol catalyst would significantly reduce H_2 cost.
- Directly related to goals; good initial analysis of catalysts; supports effort to reform bio-derived liquid fuels.
- Project supports DOE program goal of hydrogen production from renewable resources.
- Seeks to reduce cost for ethanol steam reforming by identifying base metal catalysts and thereby eliminating need for platinum-group metal catalysts.
- Project has excellent relevance to DOE H_2 Production goals.
- Identification of inexpensive (non-precious metal) catalyst is critical.
- Ethanol is only a transition fuel to the hydrogen future which cannot meet all (domestic) transportation needs and lignocellulosic ethanol production has (many technology barriers).
- Suggest looking at other biomass-derived liquids (e.g., dimethyl ether).
- Unclear as to the cost reductions achieved with $CoZrO_2$ catalyst and low temp processing but assume costs are lower than precious metal so likely helpful in reducing capital costs.
- Useful empirical validation.
- Important effort to find a metal free catalytic system.

Question 2: Approach to performing the research and development

This project was rated **3.4** on its approach.

- Too much experimental data is presented: specific approach to optimizing performance is obscured. Needs an overview to explain differences between tests conducted.
- Good initial start; good focus on reaction mechanisms.
- Sound approach based on fundamentals of heterogeneous catalysis: identify active catalytic phase(s) and synthetic techniques to optimize population of those sites; identify reactive intermediates, reaction networks and desired reaction pathways. Identify deactivation pathways and regeneration methods.
- Outstanding systematic approach to catalyst characterization and structure/property relationship.
- Firm fundamental scientific approach; strong application of catalyst characterization techniques.
- Excellent catalyst R&D. Excellent presentation of results (albeit with too many slides).
- Need systems analysis to determine if this is a viable project and to define research objectives.
- Good use of thermogravimetric and infrared analysis to follow reaction mechanism.

- Logical and well thought out approach.
- Fuel processor capital costs, O&M, and feedstock issues are addressed by this project.
- This is a university project. The approach is to select few materials, prepare catalyst, carry out reforming reaction, and study deactivation/regeneration characteristics. This seems to be quite appropriate for university-led research.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.4** based on accomplishments.

- Hard to quantify significance of test results since no longevity testing.
- Achievement of high H_2 yield at <500C is significant.
- Lifetime testing is missing. Although unknown, the performance may decline precipitously. Good initial progress, but less than half complete; quality data presented.
- Identified very active, selective cobalt-based catalyst as well as preferred support and methods of preparation.
- Comprehensive studies on characterization of bulk catalyst as well as surface intermediates.
- Good body of work on catalyst evaluation for activity, selectivity.
- Impressive property-activity correlation completed to maximize catalyst performance with minimal trial and error.
- Modified catalyst formulation has outstanding H_2 selectivity with minimal CO production.
- Outstanding application of basic science to achieve a promising commercial solution to EtOH reforming.
- Excellent understanding of catalyst performance.
- Excellent set of experiments.
- Catalyst reaction mechanism and selectivity well understood under varying temperatures.
- Need more stability data; they only have 70 hrs.
- Need a purification scheme.
- Good data; useful information to other reformer studies.
- (Good) understanding (of) the competing reaction networks in steam reforming of ethanol.
- (Good) identification of active (reaction) sites.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.6** for technology transfer and collaboration.

- No evidence of any collaboration.
- Not clear on partner roles/activities to date.
- Not at all clear what the supporting organizations (NexTech, PNNL) have contributed to this work.
- Good collaboration with catalyst manufacturer and PNNL for economic analysis.
- As catalyst technology is considered close to commercially ready, need to add an industrial collaboration.
- Could use a reactor design and reforming commercial partner.
- Should work to identify 'industrial partnerships' for catalyst scale-up.
- Industry interest is missing. Lacking active collaborations with other groups.
- Good coordination.
- Excellent body of publications and presentations. Glad to have this knowledge in the public domain.
- Teaming with NexTech Materials for catalyst manufacturing scale-up.
- Teaming with PNNL for economic analysis & catalyst deactivation studies.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.2** for proposed future work.

- Need to add long term testing.
- Strong plan, especially deactivation/regeneration studies.

- Good plans for the future builds on the group's strengths: kinetics and mechanistic studies, in-situ characterization of working catalyst surfaces, and identification of deactivation pathways. This is a new catalytic system and needs to build the fundamentals in order to advance to a commercial process.
- Must assume project partners (NexTech and PNNL) will be involved in the catalyst scale up and economic evaluation.
- Future work properly focused on deactivation/regeneration, catalyst production considerations, and overall economic analysis.
- Should develop overall process design in which to use this catalyst.
- Could this catalyst technology be used for reforming of other bio-liquids?
- Would be useful to see economics of the processor and hydrogen production (costs) as calculated using DOE's H2A model.
- Although not included on poster, assume there are plans to process other feedstocks beyond ethanol.
- Well thought out and appropriate
- Research plan for future work is very reasonable.
- Kinetic and mechanistic investigations (well) coupled with in-situ characterization.
- Economic analysis based on updated catalyst system knowledge database.

Strengths and weaknesses

Strengths
- Research may have an ethanol catalyst breakthrough but it's too early to tell.
- Good focus on reaction mechanisms.
- Excellent R&D effort.
- World-class catalyst research.
- Comprehensive reporting.
- Strong basic fundamental understanding of reaction sites. Availability of graduate students and post-docs at OSU. Lower overhead rate compared to industry and national labs.
- At this point (only 40% complete), no glaring weaknesses.

Weaknesses
- Needs description of catalyst optimization approach. What is strategy beyond experimentation?
- Needs catalyst life testing.
- No systems understanding demonstrated.
- Poster presentation did not adequately provide the means to address all the issues.
- Stronger coordination with partner(s) needed.
- Too much data presented. This much technical detail is not needed for this type of review.

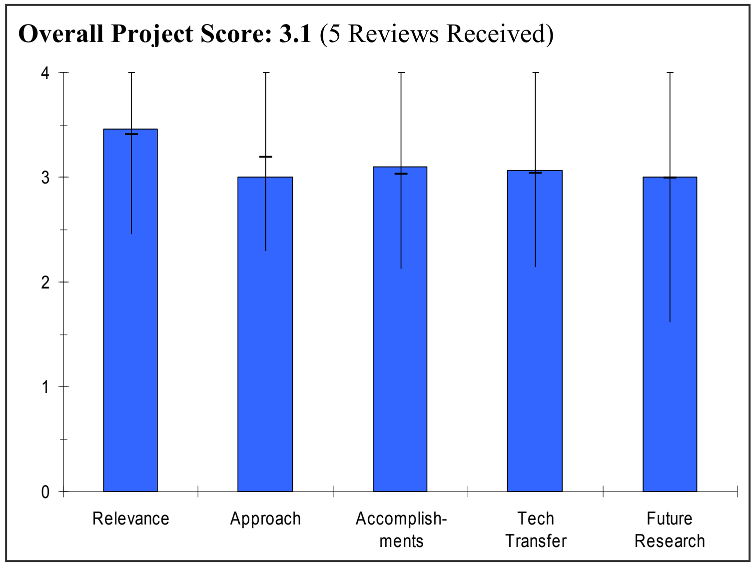
Specific recommendations and additions or deletions to the work scope

- Add catalyst lifetime testing.
- Add testing of contaminants.
- Suggest construction of integrated process development unit.
- Economic analysis should be an integral part of research in order to quantify effect of R&D achievements and steer R&D objectives.
- Continue to support the work.

Project # PDP-07: Distributed Bio-Oil Reforming
Bob Evans; NREL

Brief Summary of Project

The National Renewable Energy Laboratory is developing the necessary understanding of the process chemistry, feedstock compositional effects, reactor configuration, catalyst chemistry, deactivation, and regeneration strategy as a basis for process definition and assessment for automated distributed reforming of whole bio-oil. The objective in 2012 is to produce hydrogen for less than \$3.80/gge. The objective for 2007 is to demonstrate integration of bio-oil atomization, partial oxidation, and catalytic conversion to obtain equilibrium syngas composition at 650°C.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

- Important to further the understanding of biomass pyrolysis interactions.
- Developing a viable pathway to achieve a renewable forecourt production system is a major step forward.
- Good focus on conversion of biomass to liquid fuel to hydrogen.
- Key source of renewable hydrogen.
- Provides cost effective syngas for bioproducts.
- Supports MYPP gasification / pyrolysis technology development.
- The program focuses on developing autothermal reformer for bio-oil processing to meet DOE 2012 hydrogen cost targets for biofuel production of hydrogen. However, focus is on methanol currently not other more relevant alcohols like ethanol, sorbitol etc.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- Use of modeling in parallel with experimentation is good.
- Good focus on bio-oil conversion; unclear on whether path from biomass to bio-fuel to hydrogen makes sense from an energy cycle viewpoint.
- Addresses key thermochemical barriers to low cost syngas.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.1** based on accomplishments.

- Scale up of ultrasonic nozzle atomization not well understood/explained.
- Need to better quantify extent of sooting and degree to which it can be burned-off/cleaned.
- Reasonable progress, yet unclear if cycle is viable.
- Good accomplishments for limited budget.
- Focused on major barriers.
- Successful in developing needed analytical instrumentation / methods.

- Developed atomizer, cracking process and autothermal bench scale reactor. Validated the need for oxidation to increase CO production.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.1** for technology transfer and collaboration.

- Focused primarily on NREL activities.
- (Should) link work to thermochemical research in the Office of Biomass Programs at DOE to produce (bio)-products.
- Good representation from national lab, academic and industrial partner, yet more collaboration with industry is needed.
- Papers will be given at ACS and other public forums to share results.
- Partnership with Chevron further demonstrates project merit.
- University of Minnesota performing systematic catalyst study.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- Reasonable project but limited benefit as hydrogen pathway.
- More fundamental research should be proposed on mechanism of reactions, efficiency and catalytic selection.
- Investigators have considered contingency paths.
- Addition of WGS and parametric studies just need to broaden focus beyond methanol.

Strengths and weaknesses

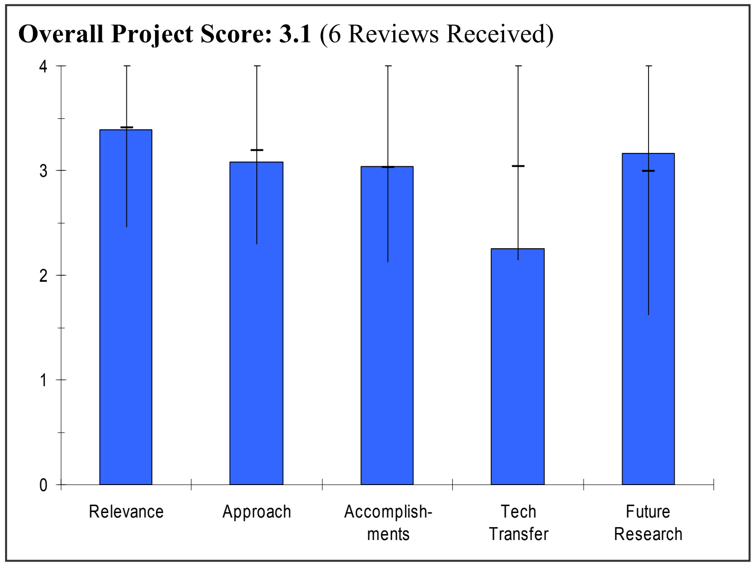
Strengths
- Tests with Rh show promise of equilibrium reaction with reversible/recoverable sooting.
- Good data on particle oxidation.

Weaknesses
- Currently requires biomass mixing with methanol. Would prefer that MeOH mixing was not needed.
- Needs more innovation and support.
- Consider an integrated bio-refinery approach to reforming bio-oils.

Specific recommendations and additions or deletions to the work scope

- Need to evaluate energy cycle.
- Independent review by company such as ADM which is heavily involved in products from oils.

Project # PDP-08: Hydrogen Generation from Biomass-Derived Carbohydrates via Aqueous-Phase Reforming Process
Randy Cortright; Virent Energy Sys.



Brief Summary of Project

The overall objectives of this project are to design a generating system that uses low-cost sugars or sugar alcohols that can meet the DOE H_2 cost target for distributed reforming of bio-derived liquids of less than \$3.00 / gge by 2017, and to fabricate and operate an integrated 10 kg H_2/day generating system. The objective for 2006 was to develop aqueous-phase reforming (APR) catalyst, reaction conditions, and a reactor suitable for converting glucose to hydrogen. Objectives for 2007 are to 1) continue to investigate catalyst, reaction conditions, and reactor suitable for converting low-cost sugars to hydrogen; 2) calculate the thermal efficiency and economics of the APR system utilizing different feedstocks (low-cost sugars, glucose, sugar alcohols); 3) compare the results of techno-economic analysis with DOE Hydrogen Program goals; 4) reach a go/no-go decision on whether to proceed with the design and construction of a 10 kg H_2/day demonstration system with the preferred feedstock; and 5) design a 10 kg H_2/day demonstration system.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.4** for its relevance to DOE objectives.

- Simple, single-step conversion of H_2 is a major step toward achieving DOE H_2 cost goals.
- Able to use renewable feedstocks.
- Strong focus on biomass conversion to hydrogen production; important pathway.
- Addresses DOE program goal of hydrogen production from renewable resources.
- Targets cost reductions in feedstocks, capital, operations, and GHG emissions.
- Small scale could provide significant advancement for renewables H_2 production.
- The objective of this project is to design and build a 10 Kg/day H_2 generating system by aqueous phase reforming (APR) bio-mass derived carbohydrates (sugar or sugar alcohols). This project is relevant to DOE's overall objectives.

Question 2: Approach to performing the research and development

This project was rated **3.1** on its approach.

- Specific approaches are proprietary. Little on which to base a score.
- Very early in the study, much of what was presented not directly linked to project.
- Continues to build on the novel concept of aqueous phase reforming as the front end of a number of biomass to fuels processes, including hydrogen.
- Work is expanding to include ever more complex sugar and sugar alcohol feeds.
- Already demonstrated that the APR can produce H_2 from glycerol and sorbitol now needs to optimize for glucose.
- Use of sorbitol or other alcohols only make sense if you are trying to maximize conversion efficiency.

- Feedstock cost, reformer capital cost, O&M, and GHG emissions are barriers addressed by this project. Due to budget cutbacks this project is focusing efforts on development of catalysts for APR.
- If feedstock costs decrease from $2.10/gge in 2012 to $1.55/gge in 2017, and hydrogen production cost are $3.80/gge by 2012 and less than $3/gge by 2017, then the approach will reach DOE's projected cost targets for hydrogen from bio-derived liquids.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- Claimed efficiency of ~78% is impressive.
- Not clear how long term testing can show steady H_2 production while gas conversion % declines significantly.
- Limited as project is early in development.
- Much work on catalyst and process development. Impressive progress for a small startup company.
- Gained a lot of knowledge from processing glycerol and sorbitol that is transferable to glucose and other polysaccharides. Still need to optimize hydrogen production efficiency and reduce Alkane by-products.
- Not much has been accomplished.
- Performance is still behind conventional reforming technology.
- Continuing to investigate catalysts for APR of glucose provided by ADM.
- Has shown catalyst lifetime of greater than a year and tested a first generation reactor system (Green Energy Machine).
- Studied effect of feed concentration. Generated hydrogen was burned for internal process use.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.3** for technology transfer and collaboration.

- Not clear on partner roles in development or milestones.
- Not clear what role partners ADM and U Wisconsin have played in the work to date.
- As this is a commercial venture they are very careful about IP protection so there appears to be limited sharing around catalyst technology and plans for generator design modifications.
- Poor communication.
- ADM is the only company interested, potentially to use a thermochemical route for corn sugar.
- Teamed with ADM and University of Wisconsin. APR process was developed at University of Wisconsin and therefore Virent is closely tied with University of Wisconsin. ADM is providing biomass derived liquids.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.2** for proposed future work.

- Good plan to include go/no-go decision point; need to include overall energy analysis and quantify benefits.
- Program on a clear path to a go/no-go decision for construction of 10 kW pilot demonstration system in 2007.
- Focus on low cost sugars and PSA development seems to be on target.
- Not clear what the R&D objectives are.
- Economics are marginal.
- Needs an independent assessment or risk assessment review.
- Future work in 2007 is focused on developing catalysts that converts glucose and sugar alcohols to hydrogen.
- Virent will also investigate hydrogenation technologies to convert both monosaccharides and polysaccharides to sugar alcohols.
- Go/no-go decision will be made for the APR technology.
- The PI has responded well to previous year reviewers' comments.

Strengths and weaknesses

Strengths
- Converter is simple and low temperature: no WGS, steam boiler, hydrodesulfurizer.
- Has clear commercialization potential if successful.
- Mentioned a commercial manufacturer, but didn't indicate who it was or if they had a market plan.
- Novel technology (APR).
- With limited funding, Virent has already built and operated a 6 NM3/hr alpha unit utilizing glycerol as feed stock.

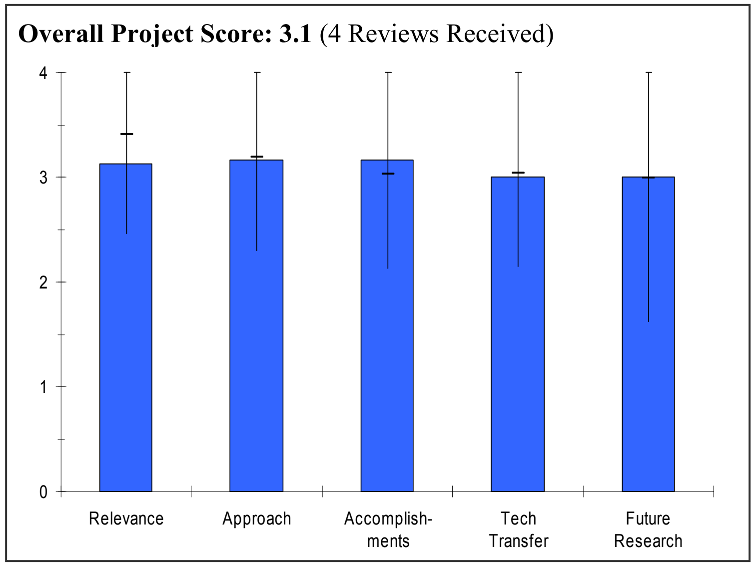
Weaknesses
- Catalyst performance degrades significantly in <1 year.
- Strategy of raising temperature to higher catalytic activity helps only slightly.
- Substantial methane production: limits H_2 yield.
- Process economics is not addressed. Should be favorable since simple, low temperature reactor, but should be quantified.
- Project is built on assumption that sugar alcohols will be available as low cost feedstocks at fuels scale The emphasis of the Virent approach should shift to a focus on low cost biomass feedstocks that might be available in significant volumes at costs under $60 per ton rather than on sugar alcohols as the US is not a major sugar producer.
- No information on commercial availability of catalyst.
- Not having a clear focus on any one particular feedstock.

Specific recommendations and additions or deletions to the work scope

- Include overall energy analysis.

Project # PDP-09: Integrated Short Contact Time Hydrogen Generator (SCPO)
Ke Liu; GE Global Research.

Brief Summary of Project



Both short contact time and steam methane reforming catalysts are being developed and a compact reforming system was designed. An interim (2006) hydrogen production cost target of $3.00/gge for distributed reforming from natural gas was achieved based on GEGR SCPO technology economic projections and those of other distributed natural gas research efforts. This project received an independent assessment verifying that the interim target was met. Specifically, GEGR is working with the University of Minnesota to: 1) discover sulfur-tolerant catalytic partial oxidation (CPO) catalysts; 2) develop sulfur-tolerant CPO catalysts; and 3) characterize CPO catalysts using X-ray diffraction and X-ray photoelectron spectroscopy. Argonne National Laboratory objectives include catalyst discovery, screening, durability testing, and characterization.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.1** for its relevance to DOE objectives.

- Development of simplified reformers, particularly multi-fuel reformers is a significant step towards meeting the DOE H_2 cost goals.
- Directly relevant to the economic production of H_2 in line with DOE Hydrogen Production targets.
- Reformer technology is critical to the initiative, but this technology doesn't appear to solve any problems or improve market penetration.

Question 2: Approach to performing the research and development

This project was rated **3.2** on its approach.

- Concept seems similar to other CPO configurations.
- Partial oxidation offers a path to compact, on site reformers, but has historically suffered from inability to operate reliably and safely at high pressure. (Good) focus on this problem as well as the identification of S-tolerant catalysts.
- Excellent leveraging of academia / national lab expertise in catalyst technology and characterization.
- Strong experimental program with impressive in-situ characterization of the reactor.
- Nothing new or innovative.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.2** based on accomplishments.

- Team has good experimental results with high space velocities.
- Great progress in operating at high pressure...a longstanding problem in this technology.
- Lots of work in evaluation of S-tolerant reforming catalyst...though not much progress towards a breakthrough.
- Successfully demonstrated applicability of short contact time hydrogen generation.

- Would be helpful to show SCPO overall process integration to produce pure hydrogen.
- Not much data presented; no comparison to conventional ATR performance.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- Impressed with strong record of collaboration with partners at U. Minnesota and Argonne National Labs. Poster clearly laid out contributions from both institutions and work processes they are using to collaborate.
- Effective collaboration between industry, national lab, and academia.
- Unclear what is being done.
- Limited publications.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- Testing at 1M space velocity is good goal.
- Not clear how practical 400psi operating pressure is: good from H_2 purification viewpoint but bad if one has to compress air/oxygen to that pressure.
- Clear path forward for natural gas reforming, and they are thinking about attacking more ambitious liquid feeds derived from renewable resources.
- Proposed future research needs to be more clearly stated.
- Would like to see a plan to commercialize this technology (start by building a prototype hydrogen generator).
- Question whether this technology can compete with conventional SMR; should capitalize on the potential to reform complex hydrocarbons which can't be done with steam reforming.
- Limited in scope and value.
- Uncertain how large cost reductions were derived.

Strengths and weaknesses

Strengths
- This is the best project I had the opportunity to review. It is using novel science and engineering to attack a difficult problem, and there is clearly a great deal of interaction and collaboration amongst the industry, national laboratory, and university participants. This is the poster child of how industry, universities, and national labs should work together in developing novel science and engineering to attack a national challenge.
- GE corporate involvement.
- Potential to handle multiple feedstocks.

Weaknesses
- Innovation.
- Independent review.
- Market study.

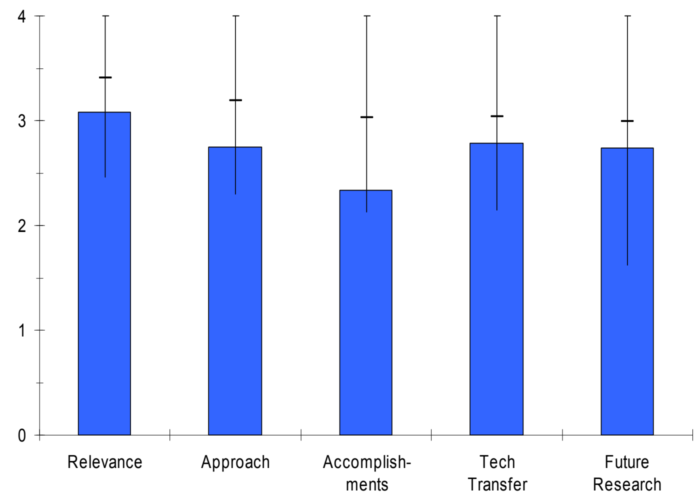
Specific recommendations and additions or deletions to the work scope

None

Project # PDP-10: Integrated Ceramic Membrane System for Hydrogen Production
Joseph Schwartz; Praxair

Brief Summary of Project

Overall Project Score: 2.7 (6 Reviews Received)



The overall objective of this project is to develop a low-cost reactive membrane based hydrogen production system that will 1) use existing natural gas infrastructure; 2) have high thermal efficiency; and 3) serve both the transportation and industrial markets – the industrial market provides immediate opportunities and will allow the project to gain valuable operating experience before fuel cell vehicles arrive. The Phase II objective is to integrate a hydrogen transport membrane (HTM) with water-gas shift (WGS) to 1) demonstrate low-cost hydrogen production, separation, and purification; 2) demonstrate HTM performance in reactive environments; and 3) develop a versatile system that can be combined with any syngas generation method for improving hydrogen production, especially at distributed scale.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.1** for its relevance to DOE objectives.

- Demonstration of process intensification is necessary to achieve DOE H_2 cost goals.
- The project is highly relevant to the production of high purity hydrogen. The work is considering membrane separation combined with WGS (process intensification). Success in either area would be of benefit to the DOE hydrogen program.
- Addresses DOE program goal of reducing capital costs in distributed hydrogen manufacture. Addresses specific barriers such as increasing membrane durability, tolerance to impurities, zero defects, high flux and selectivity.
- Integrated membrane system shows some potential for reducing hydrogen production costs.
- This is more an application engineering project.
- Scope seems to have changed from that proposed – a low cost, high performance reformer concept to meet DOE targets.
- Project objective is to develop a low-cost reactive membrane based hydrogen production system and therefore there is relevance to overall DOE objectives.

Question 2: Approach to performing the research and development

This project was rated **2.8** on its approach.

- Several concepts presented: OTM followed by HTM, and conventional reformer with HTM.
- Praxair has taken a reasonable approach. The work has focused on the development of the Zr support which appears to have been successful. In addition, they have worked on the development of alternative metal coatings (Pd and Ag). In both areas, Praxair appears to have had good success.
- Praxair has based the work on an earlier effort and has successfully leveraged the results of the prior research.
- Research at this point is primarily fundamental testing and Praxair has conducted a thorough testing program.
- The project is considering the presence of impurities. ome of the preliminary results do show some negative effect, but the Pd-Ag work does tend to indicate the material can be regenerated.
- Membrane reactors to remove hydrogen continuously during water gas shift is a sound approach to reducing size and increasing productivity of the water gas shift reactor.

- The project is relying on known materials for hydrogen separation (Pd-Cu, Pd-Ag).
- Workers recognize that thin membranes are needed to meet cost targets...wasn't clear from poster whether the membrane fabrication methods they propose to use can make these films defect free at this temperature.
- Praxair brings expertise in manufacturing the membrane substrate, with a target to do this at low cost.
- Would like to see work on thermal cycling of membranes to ensure integrity after multiple cycles.
- This project appears to have (departed from initial proposal), as it is not a high efficiency, low cost platform
- Just barely better than conventional.
- Unclear performance on wide ranges of natural gas composition.
- It appears that this particular project will not focus on reforming of natural gas (OTM) but only on HTM. Results obtained in previous DOE-funded project on OTM for reforming of NG will be used here.
- WGS catalyst might impede the performance of HTM and therefore there won't be much advantage in combining shift reaction and separation in a HTM membrane reactor.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.3** based on accomplishments.

- Total progress to date (accounting for funding delays) is good.
- Results thus far appear to be very good. Praxair is reporting that the results are meeting the DOE targets. However, reluctant to clearly present flux rate and conditions making it difficult to compare results to other work. In addition, cost information on the membranes is presented in a different format and it is not clear that they are effectively meeting the DOE targets.
- The work has resulted in the development of approximately 5 micron metal layers which is a good metal depth.
- The project has considered capital costs and the information provided suggests that this technology will improve over PSA separation.
- Prototype was developed, but not evaluated for scale-up, cost and risk.
- Manufacturing issues.
- Disappointed to see the lack of progress.
- Results are not promising for pilot plant demonstration.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.8** for technology transfer and collaboration.

- Praxair is the primary developer of the technology and is clearly interested in future commercialization of the technology. In addition, RTI has been involved in the development. This is an area that Praxair has been interested in for some time and they have a solid background in the technology development.
- Distribution of the results publicly is limited. Praxair needs to provide some additional public information. All of the data/information generated is not proprietary, and this work is of limited use to other developers and researchers.
- As membrane fabricator, RTI will be key contributor towards fabrication of modules.
- Reasonable amount of collaboration.
- Papers published, patents filed.
- Research Triangle Institute is developing Pd-based membrane for shift/separation. Praxair fabricates tubular membranes. It is not clear who is doing the catalyst work.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.7** for proposed future work.

- Future plans are somewhat vague. It appears that Praxair will continue basic testing and conduct some basic economic analysis, but it is not clear if there will be any scale-up work.
- Next key step is to fabricate modules and demonstrate WGS integrated with H_2 separations.
- Assuming success, they can move on to next key tasks: defining production methods and commercial systems.

- Proposed future work not clear or detailed enough.
- Doesn't address the issues with the technology such as durability and performance as a function of natural gas composition.
- Manufacturing defect tolerance.
- Independent assessment of risk.
- Praxair proposes to demonstrate performance in integrated WGS/HTM reactor. This will be a challenge. Effect of trace impurities in syngas on HTM is not addressed.
- Praxair plans to pursue other technology if HTM is not economical – this seems to be a good idea.

Strengths and weaknesses

Strengths
- Compelling economics if flux goals can be achieved.
- Hydrogen separation membrane appears to have good potential to effectively separate and produce high purity hydrogen streams.
- Good performance on previous projects (OTM for NG reforming) and process intensification to reduce costs.

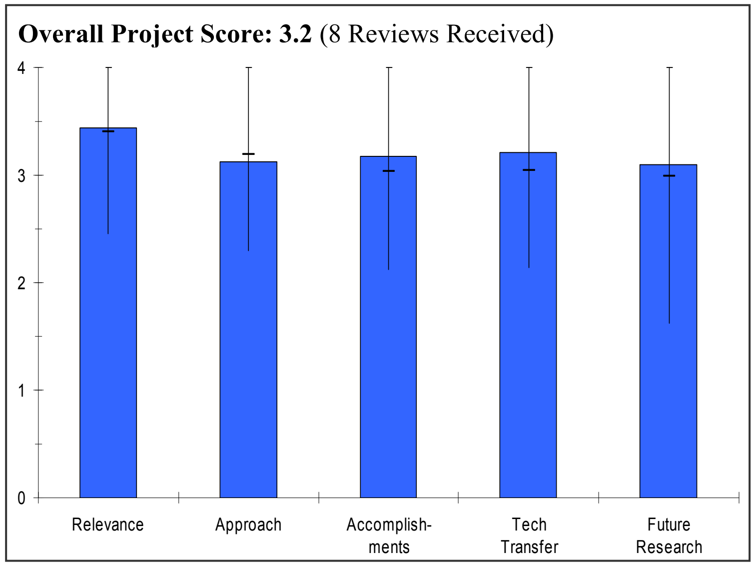
Weaknesses
- H_2 flux accomplishments not specified. Unclear why technology performance is withheld.
- Cost goals should clarify if they are per tube or for entire separation system.
- Statement in conclusion of cost goal being hard to achieve is not substantiated.
- Unclear about sulfur/other substances contaminating the membrane. Need test data.
- No significant weaknesses.
- Poster did not clearly state assumptions for the stated cost/performance benefits.
- Not cost effective.
- No clear manufacturing cost strategy to achieve DOE goals.
- Combining shift and separation steps in a HTM membrane reactor without knowing the effect of WGS catalyst on the performance of HTM in separating hydrogen.
- No studies on effects of trace impurities found in NG on HTM performance.

Specific recommendations and additions or deletions to the work scope

- Testing should be conducted with more realistic gas feed compositions.
- Independent review of cost benefits.
- Complete a risk assessment on whole development.

Project # PDP-11: High-Performance, Durable, Palladium-Alloy Membrane for Hydrogen Separation & Purification

Scott Hopkins; Pall Corp.



Brief Summary of Project

The overall objective of this project is to establish the technical and economic viability for use of a palladium alloy composite membrane in a distributed hydrogen production system. Objectives are to 1) develop a process that leverages the technical capabilities of a membrane for maximum economic benefit (reduced gallon of gas equivalent cost); 2) optimize membrane performance in terms of hydrogen throughput, purity and durability; and 3) minimize capital cost for the gas separation module, including pressure vessel, internal hardware, membrane, and substrate.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.4** for its relevance to DOE objectives.

- Demonstration of process intensification is necessary to achieve DOE H_2 cost goals.
- Pall is developing supported membranes for hydrogen separation. This is a primary DOE need for the production of pure hydrogen. The researchers are well aware of the DOE targets and are making a good effort to meet or exceed these targets.
- Pall is well aware that the membranes must move beyond a research stage and have a plan for further commercial development.
- Hydrogen separation and purification is a key element of distributed hydrogen production from natural gas and renewable fuels.
- At least for small scales of production, this approach can be cost competitive with the established PSA technology.
- One aspect of this approach is the need to establish reliability and durability, even after repeated thermal cycling.
- Technology could achieve cost and performance goals for a number of technologies.
- Permeation membranes are good. Pd-based membranes are challenged by pin-holes / thickness, hydrogen flux, poisons, and cost.
- Ties directly to the Program goal of reducing the costs of distributed hydrogen production.
- This project has the potential to reduce the capital and operating costs of distributed hydrogen production (and can also contribute to process intensification goals in the DOE Fossil Energy Hydrogen-from-Coal program).
- This project's objective is to develop durable Pd-alloy membrane for hydrogen separation.
- Development of a small, more cost effective (capital and operating) hydrogen purification system (relative to PSA) is relevant to the DOE objectives.

Question 2: Approach to performing the research and development

This project was rated **3.1** on its approach.

- Relatively simple approach that appears to have very good potential. The researchers are utilizing a porous metal tube as a support that will provide mechanical integrity. They have been able to produce membranes with

a varied pore structure capable of accepting a Zr coating that will then accept the metal layer. Metal layer thickness has been minimized (5 micron) to maximize permeation.
- The experimental approach is reasonably straightforward and they are obtaining solid data that supports the fact that these membranes are capable of separating and producing high purity hydrogen.
- Pall realizes that membrane sealing is typically a major problem and have developed an approach to overcome this problem. Their data tends to indicate that seal leakage is not an issue with the current design.
- The project approach is based on a palladium-gold composite membrane that has demonstrated high hydrogen permeance with very high separation factors at 400°C.
- The high hydrogen flux implies that a greatly reduced active surface area can be used, which, in turn, lowers the cost of the noble metals required.
- There was no discussion of a duty cycle under which the durability testing will be conducted (as listed under Future Work).
- Addresses barriers, but unclear how costs and performance will be improved.
- Pd membranes are the only known materials that conduct hydrogen exclusively thus having the potential to produce very pure hydrogen.
- Attempting to reduce cost by developing manufacturing methods with porous supports.
- The porous stainless steel tubes appear to provide a good approach for membrane supports.
- Pall will deposit defect-free Pd-alloy membrane on porous stainless steel tubes. The deposition process for the diffusion barrier layer and the active membrane material is not disclosed (proprietary?) and therefore it is difficult to judge their approach.
- Developing a small more cost effective (capital and operating) hydrogen clean up system is relevant to the DOE objectives.
- The approach to develop a compact device is especially appealing.

<u>Question 3: Technical accomplishments and progress toward project and DOE goals</u>

This project was rated **3.2** based on accomplishments.

- Achievement of flux goal is excellent.
- Achievement of weld joint Pd coverage (to avoid gas leakage) is excellent.
- Pall has produced small scale membranes that meet or exceed the DOE targets for flux and cost.
- They have been able to accomplish this with a minimal budget.
- Pall has been able to produce numerous membrane samples that all appear to be leak free.
- The larger scale membrane reactor is of a simple design and will be simple to assemble and test. In addition, it appears that membranes could be replaced with a minimal effort.
- High hydrogen permeance with high separation factors has been achieved.
- Thin membranes exceeding the hydrogen flux targets for 2005, 2010, and 2015 have been tested.
- Membrane / module fabrication techniques have been developed.
- Reproducibility of test data has been confirmed.
- Prepared tubes membrane tubes of 3/8-in diameter and 2-in long.
- Membranes as thin as 1 micron have been tested, though not at sizes above.
- Good progress on reducing the thickness of the membrane.
- High flux rates were achieved using measurements made under ideal conditions, however measurements were not made using gas streams typical of reformer gas. Effects of trace impurities on performance of membranes were not studied.
- The yield is very interesting.
- It is hoped the additional work is conducted to reduce the operating pressure down into the 100-300 psi range to relax the reformer operating cross pressures at temperature.
- It is hoped that the capital cost will be reduced or a projection thereof. The CAPEX looks to be currently ~\$2000/kg H_2.

<u>Question 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **3.2** for technology transfer and collaboration.

- Good partnership including academics, industry and a national lab. Pall is a commercial developer of other membrane systems and appears to be committed to further developing this technology. Pall is very open with the data and information generated and even if this project is not successful, the data will be of significant value to future researchers.
- The project team includes Pall Corporation, Chevron, Colorado School of Mines, and Oak Ridge National Laboratory as active participants and testing is conducted at different project sites.
- Communication appears to be lacking.
- Lacks consultation with a supplier for the stainless steel support tubes regarding cost or manufacturability issues.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.1** for proposed future work.

- Future plans including the development of larger scale membrane modules are based on larger scale modules that have been used commercially in the past, and there is a high probability that this approach will also be successful here.
- More realistic and variable gas feeds (reformate) are necessary and will be tested. For example, the membrane needs to be tested with a gas stream containing contaminants found in commercial natural gas. Currently, the data is being obtained from pure (or nearly pure) feeds which will provide some basic flux data. Mixed feed transport may be significantly different.
- Reformate should including trace species some of which may poison the membrane, before conducting optimization.
- Future work includes testing with synthetic reformate to establish operating conditions needed to achieve target performance.
- The economic analysis strategy outlined is comprehensive and should enable sound comparisons with alternative technologies, such as PSA.
- Material issues should be expanded to include more substrates.
- Longer term stability and performance.
- Planned long-term durability testing at temperature will be important.
- It is good that an economic analysis is planned as part of "future work" to estimate the cost of hydrogen production from this system.
- Other than durability testing and optimization of substrate and alloy properties, detailed future plans are lacking.
- Stated future research is rational and appropriate.

Strengths and weaknesses

Strengths
- A reasonable test project with well defined tasks. The work plan is logical and the work is progressing nicely. The project is constructed so it should be completed in a reasonable time frame.
- Good teamwork with active participants.
- Good progress towards developing gas separation modules.
- High purity.
- Good progress on flux and membrane dimensions.
- Maintaining focus on manufacturability.
- Fabrication capability.
- Pall's experience in membranes area.
- Pall's long-term relationship with ORNL.
- The yield values are very good.
- The foot print size appears to be suitable for distributed generation applications.

Weaknesses

- Unclear how the system is viable with only a 20-40 psi trans-membrane pressure differential.
- Hydrogen recovery data is not obvious. Unclear how high recovery is possible if only a <40 psi delta P.
- The work has only looked at ideal gas transport at this point.
- The work has not considered the effect of impurities in the feed.
- An economic analysis, even if preliminary, would have been helpful to provide a first-cut at the potential costs of the proposed technology.
- It would have been useful to demonstrate that the complete membrane-tube subassembly can undergo repeated thermal cycling without degradation or failure.
- Project proposes to use conventional manufacturing, has limited capabilities.
- No innovation on architecture.
- No tests yet on sulfur tolerance.
- Based on the process concept, it is unclear what the estimate is for the cost of hydrogen at 300 psi.
- No data on performance of Pd-alloy membrane using reformer gas stream.
- Unclear what will be the effect of moisture on the membranes.
- Operating pressures are a little high for SMR materials.
- Clean-up values based on Nitrogen. The effects on the likely composition of a Reformed Natural gas reformate are not discussed.

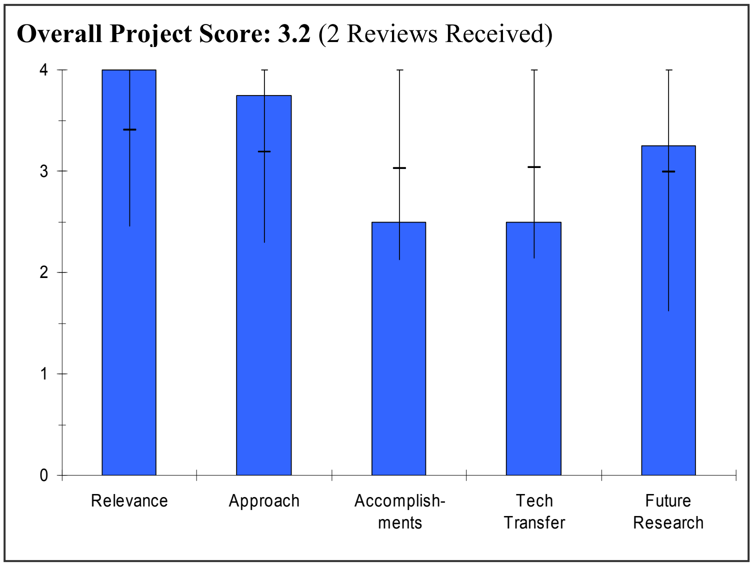
Specific recommendations and additions or deletions to the work scope

- The project is progressing nicely and needs no modifications.
- Risk assessment (is recommended) to achieve market goals.
- Economic analysis needed.
- Contaminant tolerance should be tested.
- Study the performance of the membranes in reformer gas streams (with trace impurities of sulfur, moisture, etc.).
- Evaluate the hardware for N_2, Ar, He and other trace materials that would be expected from reformed natural gas. Guidance on trace impurities is contained in the GRI Report 94/02432.2.
- Compare the results to the current thoughts on the quality needs for the vehicle OEMs. The current thinking is in a Technical Information Report Number J2719 published in 2005 by SAE. This report will be revised as additional data from fuel providers and OEMs becomes available.

Project # PDP-16: Advanced Alkaline Electrolysis
Richard Bourgeois; GE Global Res.

Brief Summary of Project

The overall objective of this project is to study the feasibility of using alkaline electrolysis technology with current-generation nuclear power for large-scale hydrogen production. Objectives are to 1) conduct a market study of existing industrial H_2 users to determine economic feasibility; 2) develop a pressurized low-cost electrolyzer to determine technical feasibility; 3) demonstrate the electrolyzer on a small scale, 4) create a design for a large scale system and 5) conduct an environmental and regulatory impact assessment to address codes and safety concerns.



Question 1: Relevance to overall DOE objectives

This project earned a score of **4.0** for its relevance to DOE objectives.

- The low cost electrolyzer technology being developed will be applicable to any electric energy source.
- Low cost electrolyzer technology is crucial to the viability of hydrogen from renewables.
- Electrolysis is one of the two most viable options for distributed hydrogen production in the near term. The problem is capital cost and cost of electricity. This project is most heavily focused on lowering the capital cost through use of GE plastics and advanced manufacturing.

Question 2: Approach to performing the research and development

This project was rated **3.8** on its approach.

- Emphasis now is on low cost manufacturing of cell stacks. The balance of plant system costs have not yet been critically examined, but will be addressed in a later phase.
- Good approach to examining existing hydrogen markets to identify potential electrolytic hydrogen customers. This could enable the development of distributed electrolysis system technologies while hydrogen demand from the transportation sector evolves.
- GE plastics are used to make individual cells with weld prep by injection molding. The individual cells are then manually combined to make the electrolyzer stack.
- No one has ever made an electrolyzer out of plastics. This necessitates a study of materials degradation which is being pursued in this project
- Accelerated testing is being done using higher pressures with a 10 year stack life as the goal.
- Part count reduction is big part of this project and a key to reducing stack cost to under $100/kW goal.
- Match to nuclear will possibly utilize low cost electricity.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.5** based on accomplishments.

- Stack costs are estimated to be $100/kW based on price quotes for all materials. A complete operating stack has not yet been built and tested.

- Balance of plant system costs have not yet been critically examined, but will be addressed in a later phase. They are currently estimated to be about $300/kW. Thus, the total system cost is expected to be right at the DOE target of $400/kW.
- Significant progress has been made on defining market and requirements.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.5** for technology transfer and collaboration.

- Most of the work appears to be GE's alone, not surprising because of the intellectual property involved.
- Involvement with Entergy is focused on NRC siting qualification and access to hydrogen customers.
- Good set of partners on this work that effectively leverages expertise.
- Proprietary information will hamper dissemination of information.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.3** for proposed future work.

- GE is taking steps to scale their technology up to 1MW+ sized systems. Reducing the relative costs of power electronics and balance of plant systems is an important step they are taking.
- It is likely that because of the plastic architecture that only modest electrochemical compression can be accomplished with this technology. This may mandate that the cost of external compression be reduced in order to make the technology economically viable.
- Future work includes building and testing a 10-cell stack in 2007, followed by conceptual design of reference plants in 2008.

Strengths and weaknesses

Strengths
- Development of technology that has the possibility for larger scale electrolytic hydrogen production today that is not dependent on the evolution of the hydrogen transportation market, but at the same time allows the development of the necessary infrastructure should the transportation market demand accelerate.
- Technology potentially amenable to mass manufacturing and low part count, reducing stack cost.

Weaknesses
- They have not built and tested devices to prove their thinking, but intend to do so in the next year.
- It will be difficult to pressurize hydrogen electrochemically to a useful pressure thus eliminating external compression requirements.
- Plastic degradation in alkaline electrolyte is potentially a problem that must be resolved.

Specific recommendations and additions or deletions to the work scope

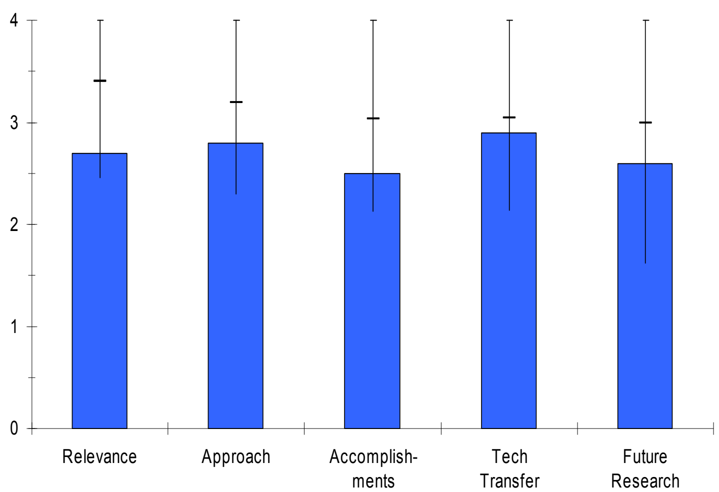
- Evaluate potential safety issues resulting from degradation of plastic materials used in construction.

Project # PDP-17: EVermont Renewable Hydrogen Production and Transportation Fueling System
Harold Garabedian; EVermont, Inc.

Brief Summary of Project

The overall objective of this project is to develop and test advanced proton exchange membrane (PEM) electrolysis fueling station technology. The objectives for this project were to 1) complete integrated system tests in-house, 2) build a public hydrogen refueling station, 3) procure a hydrogen-fueled vehicle, and 4) monitor the performance of the refueling site and hydrogen fueled vehicle.

Overall Project Score: 2.7 (5 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **2.7** for its relevance to DOE objectives.

- Any experience gained with electrolytic hydrogen production and vehicle fueling will provide useful information for future distributed hydrogen transportation applications.
- Linkage to renewable energy is weak since they simply take power off the grid whenever they need it, independent of whether or not the wind is blowing, and they purchase Renewable Energy Credits to offset any emissions that might be created from the grid sources.
- The key objective appears to be testing new electrolysis stack technology under cold weather conditions with a secondary emphasis on production of electricity to the grid for green energy credits.
- Demonstration of refueling station in cold climate is important for implementation of the hydrogen economy.
- This project installed a PEM electrolysis system as a demonstration unit, but did not produce publicly available data that will help in achieving the DOE goal of reducing the cost of distributed production of hydrogen from distributed electrolysis at the pump.
- The vehicle tested was a hydrogen ICE, so is not applicable to the program's goal of developing fuel cell vehicle technology.

Question 2: Approach to performing the research and development

This project was rated **2.8** on its approach.

- Seem to have a reasonable grasp of the technical barriers as they apply to the very small scale.
- Since hydrogen is only produced when they need to fill the tank of their one vehicle, not much is learned from stressing the system. They essentially turn the system off until just prior to a refueling event.
- Location provides good opportunity for cold weather durability testing.
- Only one vehicle fuels at the station a couple of times per week so difficult to test full reliability of components.
- The inexperience with wind turbine technology leads to suboptimal location of the turbine and wind capacity.
- Project uses a Proton Hogan 240 electrolyzer for hydrogen production to demonstrate distributed hydrogen production and refueling of a Prius ICE in a cold climate.
- This is an applied project: there is no stated objective of new materials or design development.
- Operation of the unit in a cold weather environment could provide useful information, but no data is presented on how the problems were addressed by Proton Energy.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.5** based on accomplishments.

- They built a refueling station, which has been done before.
- There was no discussion of the barriers they were supposed to address, no discussion of costs, efficiencies or lessons learned.
- Seem to be meeting project milestones and addressing cold weather issues as applicable to their system.
- Improved electrolyzer for cold weather stability.
- Learnings applied to future electrolyzer and dispenser design.
- Refueling station opened in July 2006. Hydrogen is generated at 150 psi, with compression to 5000 psi for refueling.
- The PI claims that "many enhancements" were incorporated into the electrolyzer as a result of lessons learned resulting in improved cold temperature operation, more efficient Advanced Cell Stack, improved power conservation, and easier field installation. No specific data were provided to support these claims. It is difficult to assess the true accomplishments of this project and what unique information is offered to the field.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.9** for technology transfer and collaboration.

- They did provide feed back to their suppliers to improve the balance of plant components.
- Good partnerships have permitted systems to be integrated fairly well.
- Feedback to Proton on performance of the Hogan electrolyzer is valuable from a system design standpoint.
- No collaboration or information sharing on technical advances beyond the electrolyzer manufacturer that participated in the project.
- Good collaboration with local authorities and electric utility for system siting, permitting, construction and operation.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.6** for proposed future work.

- The future plans are minimal. They have just built the refueling station, now what?
- Little remains in their project work scope.
- Performance monitoring and testing will continue.
- The project is scheduled for completion in September 2007 and future work only includes "testing, monitoring and analysis". To the degree possible, the PI and subcontractors should include in their final report data on problems encountered and how they were addressed, including more specifics on electrolyzer performance improvements.

Strengths and weaknesses

Strengths
- They have worked through the permitting and built an operating hydrogen refueling station.
- They interacted well with their partners.
- Integrated distributed electrolysis fueling system and hydrogen vehicle facilitates holistic learning.
- Project has a desirable public education feature-lots of citizens have visited and learned more about hydrogen.
- Feedback to Proton on electrolyzer design.
- Lessons learned on siting and permitting also valuable.

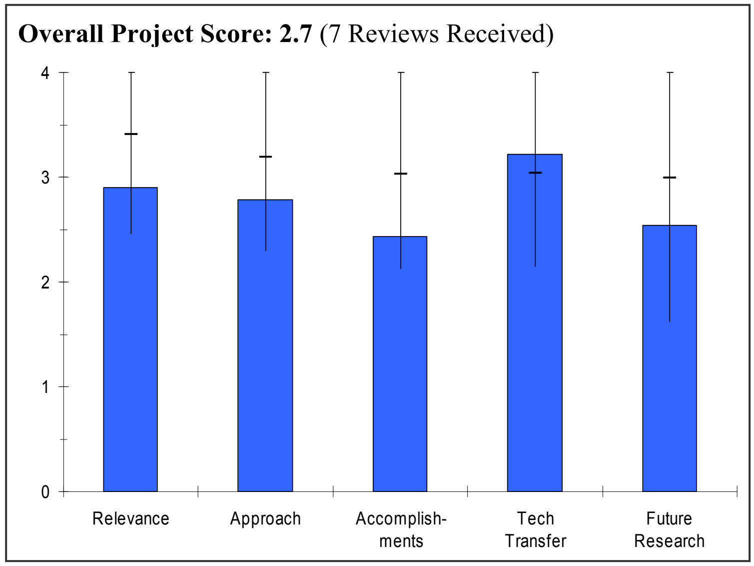
Weaknesses
- There was no discussion of cost, efficiencies, or other barriers that the DOE needs to have addressed.
- Scale and limited system performance requirements do not really test expected real world system demands.
- Linkage to renewable energy is weak since they simply take power off the grid whenever they need it, independent of whether or not the wind is blowing, and they purchase Renewable Energy Credits to offset any emissions that might be created from the grid sources.
- Not much novelty intrinsic to project.

Specific recommendations and additions or deletions to the work scope

- They should include a "lessons learned" report to the DOE which identifies areas in getting permits, balance of plant, and other lessons.
- They should be able to discuss the costs and validate the cost targets.

Project # PDP-19: Hydrogen Regional Infrastructure Program in Pennsylvania
David Moyer; Concurrent Tech. Corp

Brief Summary of Project



This is a large multi-year project that includes efforts on hydrogen pipelines, off-board hydrogen storage tanks, hydrogen separations and purification, hydrogen sensors, and hydrogen production and delivery scenario analyses. The current production and delivery analyses objectives of this project are to 1) analyze tradeoffs between alternative H_2 production and delivery approaches using commercial and near-commercial options; 2) evaluate economic delivery scenarios for the I-95 Corridor and assess the feasibility of hydrogen infrastructure along the I-95 Corridor; and 3) determine Pennsylvania's economic delivery scenarios using regional cost of indigenous energy resources (i.e., coal, landfill methane, biofuels, wind, water, municipal waste, anaerobic digestion and nuclear) using the DOE H2A Production and Delivery Models.

Question 1: Relevance to overall DOE objectives

This project earned a score of **2.9** for its relevance to DOE objectives.

- Hydrogen sensor, separation, and storage are applicable to the DOE hydrogen plan.
- Addresses DOE program goals of overcoming infrastructure barriers for hydrogen as a transportation fuel. Encompasses range of topics including local infrastructure model for I-95 corridor, hydrogen embrittlement for pipeline steels, hydrogen storage tanks for retail stations, hydrogen separations, and hydrogen sensors.
- Focused mostly on getting info on PA.
- Science already in other program projects.
- The project is divided into several sub elements, most of which have good relevance to the overall DOE objectives.
- The work on sensors is more of vendor evaluation then technology development – does not help much in progressing the hydrogen program.
- Further quantification is needed for the goals and deliverables of each subtask within this project.
- The project has three components: i) the Pennsylvania hydrogen delivery study. This component has reached a level of development that is noteworthy and should definitely be pursued further; ii) materials testing in the presence of hydrogen. This component is at an initial stage; and iii) hydrogen sensors. Definitely all three components are relevant to the hydrogen economy and support the President's initiative and the DOE R&D objectives. In particular, I would rate component (i) with a solid 4.
- This is a broad project that addresses several features of the hydrogen delivery infrastructure, and will produce some generally useful data in this regard.
- The analysis of hydrogen production and delivery options in Pennsylvania provides a useful analytical methodology for incorporating more regional analysis capabilities into the DOE's production and delivery modeling efforts.
- Overall cost of the project to DOE is high; continuing efforts are needed to make this work broadly applicable to the delivery program.
- Project consists of four parts:
  1) Pennsylvania infrastructure: results of little generalization ability to remainder of the country
  2) Pipeline and vessel materials: similar to other DOE projects

3) Separation of H_2 transported by CH_4 / H_2 mixture: PSA development
4) H_2 sensor development: DOE H_2 Production Tech Team (HPTT) recommended focus on cost of sensors being highest sensor priority, but project focuses on reliability.

- Parts lack strong focus on highest priority, core goals in MYPP.

Question 2: Approach to performing the research and development

This project was rated **2.8** on its approach.

- The work seems redundant to other work being done.
- The hydrogen separation and storage work does not seem original.
- Validation of the H2A model is useful.
- This project is really a potpourri of five smaller projects.
- The hydrogen infrastructure study for PA is interesting, but I am not sure what it tells me. It proposes to analyze the costs and energy sources for hydrogen production and delivery to serve the I-95 corridor, but that presupposes that a retail net limited to this corridor would generate a strong customer base for hydrogen fuel cell vehicles. That assumption needs to be tested—a market research assessment of driver comfort with such a limited infrastructure should precede the work reported here.
- The embrittlement study is fine as far as it goes...but would like to see more work on materials research to address the strain/embrittlement issue for the Heat Affected Zone (HAZ).
- H_2 separations: it's not clear how this fits in with the other projects. Also, private industry is putting a lot of effort into hydrogen PSA technology, and it is not clear to this reviewer why the DOE has to support research in this area.
- H_2 Sensors: I understand importance of this work, but it seems to me that the studies reported here should be the responsibility of developers of hydrogen sensors as part of the qualification of their products.
- Reasonable approach – segmenting into 3 parts
- Looked only at politically correct feedstocks – mainly coal.
- Approach taken by the pipeline and storage subtask is good – involves providing good direction to the collaborators and selecting the right set of tests. Similar implementation is lacking for the infrastructure study and separations & sensors subtask.
- The infrastructure study subtask will do good to seek the industry input on expected timelines for expected FCV and station rollout scenarios.
- Application of the H2A Production and Delivery Models in Pennsylvania is a unique effort addressing the barriers that a multiple urban and county region setting poses on hydrogen delivery. The approach of limited resources and transportation of the energy carrier from the western part of the State to the metropolitan centers at the eastern part is very pragmatic and addresses real world scenarios. Also the implementation of the current coal cost to the study is extremely relevant since it corrects optimistic scenarios for natural gas feedstocks involved in the H2A approach. Lastly, the study of the refueling locations along the I-95 corridor will provide a great tool for attacking the problem of implementing the hydrogen economy in a way friendly to the public. The results of this project will provide a valuable tool to the DOE on the implementation of the hydrogen economy in a way that addresses specific regional and state demands.
- Testing of materials and pipeline components against hydrogen failure and identifying the sources of failure is a critical step toward achieving hydrogen material compatibility. The work carried out at SRNL is of good quality and should continue. An interesting part of the work is the testing of the Composite Over wrapped Pressure Vessel (COPV). Burst and fatigue testing is the right approach to validate the viability of these composite structures (aluminum liner wrapped with carbon fibers) intended to be used for hydrogen storage.
- Certainly hydrogen sensors are a vital part of the hydrogen project. It seems that the work has identified hydrogen contamination as a serious source of errors in hydrogen sensing and suggested sensor A and C designs (after they were modified by the manufacturer) as possible ways to improve resistance against degradation. The issue of sensors is an important one, but it is not clear what the overall approach is. For instance, why were sensor types A, B, and C the ones tested and not another sensor, say, D?
- Good to see that the task on developing Type III COPVs for off-board storage will be focused on meeting DOE cost goals.
- PI of the Sensor task should ensure that the project is consistent with the hydrogen quality guidelines being developed by SAE.

- Research focuses on PSA adsorbents and sensor reliability, when refinery PSA operators' priorities are valve reliability and fueling station developers are requesting cheaper sensors.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.4** based on accomplishments.

- Did not show significant accomplishments to overcome the barriers that were to be addressed.
- For money/budget results could be better. Why are sensors, adsorbents, and burst pressure of storage vessels key challenges for H_2 in PA?
- The progress is slow and very little was accomplished in the area of infrastructure study and RPSA development.
- The accomplishment in the sensors field was to develop a more S tolerant sensor, which can be useful.
- Have revised the goals for the storage subtasks to off-board storage with focus on cost reduction. The goal is quite relevant to current needs, however late realization in terms of revising the goal.
- Good progress on the pipeline subtasks, with the right choice of test matrix.
- Progress in component (i) (The Pennsylvania hydrogen delivery study) is outstanding. The project clearly identified key issues with the H2A approach and expanded on their use and applicability. The analysis of the delivered hydrogen cost as it relates to the increase in the coal feedstock price is a successful one. Similarly the hydrogen delivery cost for 1% demand along the I-95 corridor is a significant one. Again, I rate the accomplishments of this component with a solid 4.
- Progress on materials testing in the presence of hydrogen is summarized by the stress-strain curves of HAZ and weld metal materials, as well as by the fabrication and testing of the COPV. In particular, the fact that the HAZ exhibits a smaller ductility in the presence of hydrogen relative to the base metal and welds is a good technical result.
- Progress on sensor testing can be summarized by the slide titled "Modified Sensor Test Results." A good description of the sensing capabilities of designs A and C.
- Appreciate that an initial cost estimate was provided for the COPV tank.
- Given the high level of funding authorized for this effort, especially relative to the size of the total Delivery program budget, the overall accomplishments are not especially significant.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.2** for technology transfer and collaboration.

- There was good interaction with sensor companies.
- The coordination between various efforts on the codes and standards was good.
- Close collaboration of Concurrent Technologies with wide range of collaborators is apparent.
- Many collaborators but not clear how much they are learning from other programs — for example, separations program looks identical to other projects funded by the Program or work going on at PSA vendors.
- Good collaboration between diverse team members and different sub elements.
- Technology Transfer is the highlight of this project as it involves directly engaging the vendors who will later commercialize the technology.
- The Pennsylvania study component is interfacing with the developers of the H2A tool and contributes significantly to its (H2A) applicability both at a state and intra-state level. The planned interactions with the stakeholders is a good approach as it will allow for real-world input and at the same time the public will be given an opportunity to be educated on the structure of the hydrogen economy and its impact on cities, counties, and states.
- The hydrogen-materials testing is interfacing with ASME. The project can become a valuable source of information to the effort for the development of codes and standards.
- It seems that the sensor-component of the project is interacting with sensor manufacturers. However, the extent of this interaction is not clear. Also it is not clear what the importance of this interaction to the viability of the project is. Is the project providing the manufacturers with key new ideas or is it just testing and modifying existing technologies?

- Good collaboration with Pipeline Working Group (including ASME and SRNL) on pipeline embrittlement tasks.
- Broad group of academic, institutional and industrial partners.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.5** for proposed future work.

- They need more definition on how they are going to overcome the final barriers that they identified.
- As noted above, future infrastructure work should begin with a market survey study to define consumer expectations for availability of fueling stations. Recent studies I have seen suggest auto buyers want to see fuels available at 40% of the retail stations before they will purchase a vehicle that requires a new fuel. UC Davis studies say the figure is 10%. The discrepancy needs to be resolved before we assume the 10% figure is valid and forms the basis for an infrastructure modeling study.
- Materials for pipelines: put more focus on metallurgy and new materials concepts to address embrittlement in HAZ
- Composite H_2 storage vessels: Lots of work on this being done by private sector companies. Not clear why the DOE should be supporting work that competes with these efforts. Are there really novel approaches in the DOE funded programs that promise significant advantages over the current commercial approaches? I didn't see them in the poster.
- Rapid cycle PSA. Air Products and Questair are working on this for other applications. Not clear to me why this needs DOE funds to ensure new concepts and materials are being developed.
- Proposed future research is adequate to meet the said objectives of the project.
- Articulation of specific targets for individual elements of the project will help in assessing the merits of proposed future research.
- Again, the Pennsylvania hydrogen delivery study component has a well thought out plan for future research. In particular the consideration to meet with stakeholders for possible input seems to be an approach in the right direction. This input is extremely important to both the Pennsylvania energy options and the establishment of the hydrogen economy along the I-95 corridor.
- Proposed research on off-board hydrogen storage is in line with DOE goals. Mechanical testing of material components of COPV is needed to ascertain possible ways of improvement of the COPV capabilities. However, it is not clear what the proposed serviceability modeling of the COPV entails. There is no information to judge the objectives and potentials of this modeling.
- The proposed identification of emerging sensor technologies from universities and national laboratories is a proper task but seems too broad. Perhaps some metrics that would assist this identification ought to have been stated. Also the design and construction of the intrinsically safe package to contain safety hydrogen leak sensor system is a rather vague one. A few details on how one can achieve this objective would help elucidate whether the proposers are moving in the right directions toward such a design.
- Significant cost reductions are needed for the COPV tank in order to meet DOE cost goals, and potential pathways for achieving the cost reductions should be described.
- Continue to seek ways to add value to the delivery program and provide results that have broad relevance and impact.
- Future sensor work addresses packaging and contamination issues, not cost.
- PSA work does not address reliability issues with PSA's, especially valves that are a concern for pipeline situations where reliability is critical.

Strengths and weaknesses

Strengths
- Good team interactions.
- The progress has improved over previous years.
- Good relevance to DOE’s technical and portfolio goals.
- Directly working with vendors who will potentially commercialize the technology.

- The Pennsylvania hydrogen delivery studies are indeed a significant effort that needs to be supported and encouraged to continue. The poster presenter, Eileen Schuma, did an excellent job in pointing out the strengths of the project and its potential impact on the I-95 region and its environment.
- The collaboration with the SRNL on materials testing is a good approach since SRNL has good capabilities of carrying out high quality work on hydrogen-induced degradation. The COPV project is a promising technology that should be supported and further explored.
- The people behind the project: Eileen Schuma has a continued and successful participation in the Pennsylvania delivery component; I do not know for how long David Moyer is involved in the project, but it seems that he understands well the overall project directions.

Weaknesses

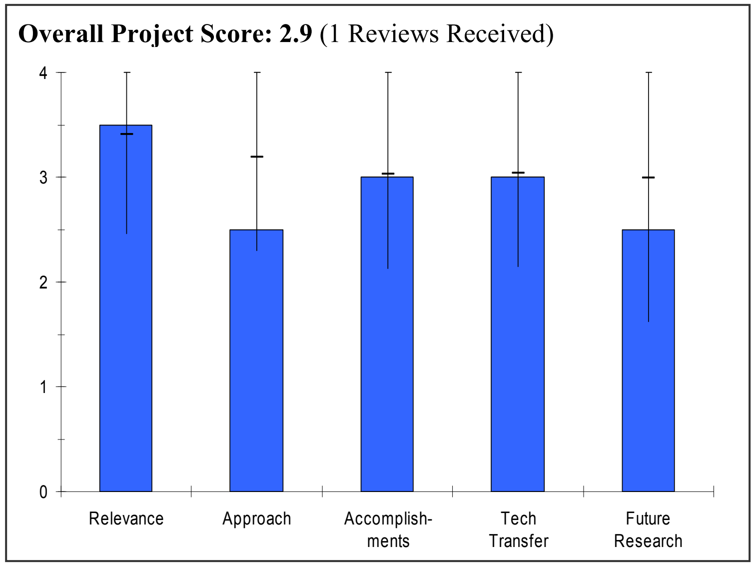
- The model validation is for a small area of the US. They should have included more than just the I-95 corridor.
- The separation work is not innovative.
- As an earmarked program, not clear how much collaborating they are doing with other programs.
- There are several subtasks/projects with little or no relevance to each other. They can probably be separated into different projects for better assessment.
- Materials testing should become more focused and coordinated. Perhaps a close collaboration with ASME will help identify the types of tests required to increase our understanding on material failure, and hence help in the direction of establishing a design methodology.
- Regarding the sensor component, I may say that the poster did not provide enough information. For instance, it is not clear what the underlying science for sensor reliability is and how the palladium degradation can be avoided. It seems that much more work is needed in this direction or else this component of the project runs the risk of being typecast as one in which sensors are tested randomly and the ones performing better are selected.

Specific recommendations and additions or deletions to the work scope

- They need to show how their infrastructure analysis applies to other parts of the country.
- They need to compare their PSA results with DOE targets and with other work in the area.
- The work on sensors should be eliminated. It has little or no relevance to other project elements and is something that a vendor might be able to sort out himself.
- For the materials testing, sharing of the results with the rest of the members of the pipeline working group is an efficient approach toward establishing a scientific exchange and perhaps a better coordination on identifying new critical tests that need to be conducted.

Project # PDP-23: Evaluation of Alternative Thermochemical Cycles
Michele Lewis; ANL

Brief Summary of Project



The objective of this project is to balance the temperature portfolio of nuclear heating sources with thermochemical cycles for H_2 generation, using the Gen IV Energy Conversion Program for electrical generation and the Nuclear Hydrogen Initiative (NHI) for hydrogen production. The approach will 1) identify promising cycles from the literature with various maximum temperatures to match heat output from different nuclear reactors; 2) invite university participation to evaluate cycles using consistent methodology – universities include Clemson, Howard, Massachusetts Institute of Technology, Pennsylvania State University, Rensselaer Polytechnic Institute, Tulane, University of South Carolina, University of Illinois-Chicago; 3) determine critical research and development (R&D) needs or recommend no further work; and 4) down select 1 or 2 of the most promising cycles for further R&D. The NHI methodology consists of 3 levels of evaluation:

- Level 1 based on stoichiometric reactions;
- Level 2 based on equilibrium considerations;
- Level 3 based on 'real' chemistry to the extent it is known;
- Pinch analysis used for heat management in all levels.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

- Project builds on prior research and is focused on identifying alternative thermochemical processes.

Question 2: Approach to performing the research and development

This project was rated **2.5** on its approach.

- Uniform evaluation of processes is a good approach.
- Laboratories involved in the project should review each other's work and validate results to verify as appropriate and feasible the most promising and/or most difficult processes.
- A basic cost/benefit analysis (e.g., basic H2A cost analysis or scoring method) for evaluating the benefit of processes that create less challenging environments (e.g., are less corrosive), require fewer unit operations, or less complex process equipment should be included in the evaluation of the processes.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- Not all processes have been evaluated at the same level of technology maturity, which may impact final evaluation

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- Very good use of university collaborations.
- Industry expert input into the potential materials, manufacturing, or other implementation problems would be very helpful.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.5** for proposed future work.

- All processes should be brought, as nearly as possible, to the same level of experimental (laboratory scale) development prior to selecting most promising candidates.
- Considerations other than efficiency should be included in the down-select of promising processes.

Strengths and weaknesses

Strengths
- Excellent use of university talent.

Weaknesses
- Need to consider additional attributes of processes to fully address DOE needs.

Specific recommendations and additions or deletions to the work scope

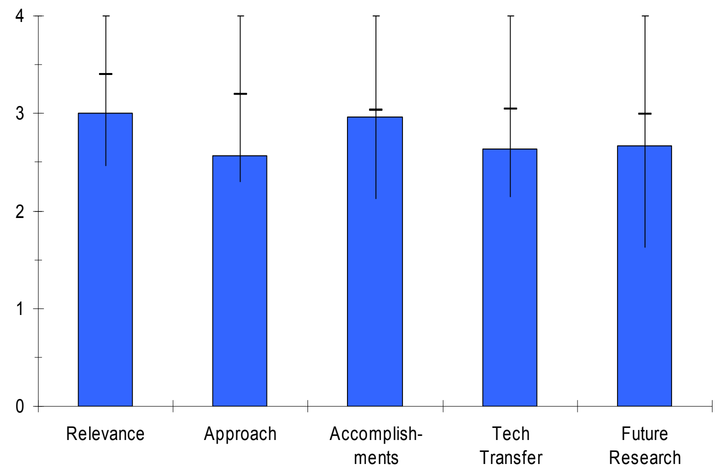
- Add cost/benefit analysis.

Project # PDP-24: UNLV High Temperature Heat Exchanger Development
Tony Hechanova; UNLV

Brief Summary of Project

The objective of this project is to assist DOE-NE in the development of hydrogen production from nuclear energy through:
•Identification and testing of candidate materials and coolants for heat exchanger components.
•Design of critical components in the interface and sulfur iodine thermochemical process.
•Fabrication and testing of prototypical components.
•Innovative materials development.

Overall Project Score: 2.8 (3 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.0** for its relevance to DOE objectives.

- This project is funded through the Nuclear Hydrogen Initiative. The objective of this project is to assist DOE-NE in the development of hydrogen production from nuclear energy through identification and testing of candidate materials and coolants for heat exchanger components and for thermochemical reactions.
- Project addresses key issues in the Nuclear Hydrogen Initiative, but closer coordination with specific needs of process and equipment developers should be pursued.
- This poster covered nine individual tasks of relevance to the Nuclear Hydrogen Initiative. As such it covered a range of topics, each quite briefly.
- It is apparent that the researchers have worked with the rest of the NHI to make their individual tasks as relevant as possible to the on-going work.

Question 2: Approach to performing the research and development

This project was rated **2.6** on its approach.

- The objective of this project is to evaluate the performance of large number of materials for production of hydrogen from nuclear sources. Several team members are involved in this project and it appears each one is doing research on their own.
- Several different experiments are used in this project.
- This project consists of several mini-projects and there is no connection between them.
- The work is focused on the barriers to the implementation of the thermochemical hydrogen production cycles, including corrosion, heat transfer in the heat exchanger and the development of catalytic materials.
- The sensitivity shown for Task 5 was quite impressive, but it is unclear how that work will be applied to the issues of electrolytic cells. The listed accomplishments state the measurements that were done, but don't draw any inferences or conclusions.
- A tighter program management system with better-defined objectives and milestones for each task is required. If this exists, it was not apparent from the information presented.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- Corrosion and crack growth studies were carried out.

- Properties of materials were studied after exposure to acidic conditions.
- Candidate materials were examined for HI decomposition.
- Some mechanical property measurements were carried out.
- There is a wide range of progress among the nine tasks. Some appear to be just getting underway, while others seem to be well advanced.
- Same good technical progress was made, but it was hard to evaluate how much progress was made toward specific goals and overall project needs.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.6** for technology transfer and collaboration.

- Partners in this project are: UNLV, UC Berkeley, MIT, General Atomics, Ceramatec, and Argonne. It is not clear if any coordination exists among the team members.
- There is evidently a good deal of collaboration between the Nuclear Hydrogen Initiative and the tasks. It is not clear whether the technology transfer is from UNLV to the other NHI participants, or from those participants to UNLV.
- Better collaboration between university researchers and process developers (industry and national labs) should be incorporated. This will help to ensure that the research addresses specific needs, such as operating conditions and other requirements.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.7** for proposed future work.

- Proposed work lists lots of tasks.
- Tasks are relevant to Nuclear Hydrogen Initiative.
- Looks like this team is shooting in the dark—hoping they will hit a star!
- The scope of future work appears to be much more aggressive than the scope of work accomplished to date, even though the work has been underway since 2003. Perhaps this is more a mark of optimism about future successes than a realistic evaluation of what can be accomplished in the next year or two.
- There is not future work listed for Task 5. Will this work continue?

Strengths and weaknesses

Strengths
- Fairly big research team.
- Has significant amount of funding.
- Facilities to carry out various tasks are available.
- The tasks span a wide range of the issues confronting the development of thermochemical cycles for hydrogen production.
- The university seems to have a wide range of new equipment at its disposal for the investigation of material properties.

Weaknesses
- Lack of real collaboration among team members.
- Lack of focus.
- It is not clear if the results of the research are being given to the rest of the NHI participants in a timely manner to influence choices of materials and other issues.
- Project seems to lack a sharp focus and a good definition of specific goals and objectives.

Specific recommendations and additions or deletions to the work scope

- Define two or three problems and develop a plan of attack.
- Recommend that the tasks be structured to include work to understand and fix identified problems and not merely to take pictures of the problems.

Project # PDP-26: Test of High Temperature Electrolysis Integrated Laboratory Scale Half Module

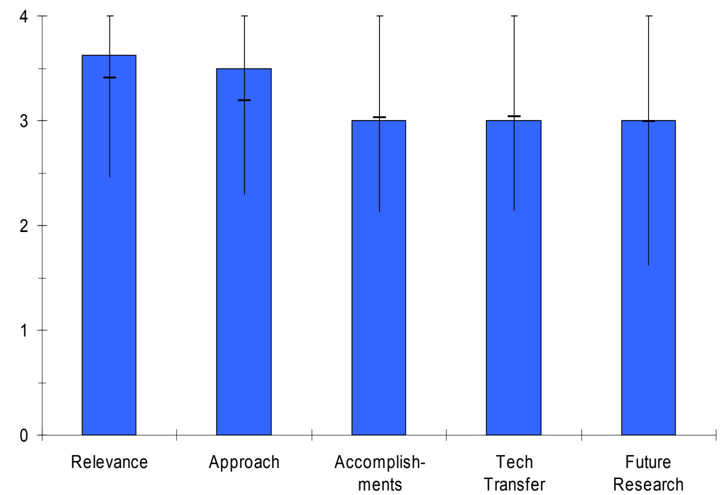
Joe Hartvigsen; Ceramatec

Brief Summary of Project

The objective of this project is to test an integrated laboratory scale (ILS) hydrogen production module. The "Half-ILS Module" test at Ceramatec will achieve the following:

- Development and testing of two 60 cell stacks in similar configuration to a full module;
- Show that performance scales with stack height;
- Assess system issues with stacks;
- Develop component production capacity (100 cells/month);
- Deliver first full ILS module to INL.

Overall Project Score: 3.2 (4 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.6** for its relevance to DOE objectives.

- High temperature electrolysis is important to improving electrolytic efficiencies in large central hydrogen production facilities.
- High temperature electrolysis can be used in advanced nuclear and solar thermal applications, which are both carbon free.
- The hydrogen produced can also be used to produce carbon based fuels by hydrogenating CO_2 emissions from power plants or other CO_2 sources, and the high temperature oxygen byproduct can be used in biomass applications.
- This project is concerned with the development of high temperature steam electrolyzer (HTSE or SOEC) for use in nuclear hydrogen production.
- High temperature solid oxide electrolyzers have greater efficiencies than lower temperature electrolyzers; however, the materials issues are much greater. They match up well with nuclear.
- Good work.
- Not clear how SOEC cost compares to targeted electrolyzer cost.
- Development of high temperature electrolysis is a major option for hydrogen production by water splitting using advanced nuclear reactors. This project is an essential part of that development program.

Question 2: Approach to performing the research and development

This project was rated **3.5** on its approach.

- They seem to have a reasonable grasp of the technical barriers. Seals that perform well in high temperature environments seem to be one of the most significant since they limit the pressure drop across the plates. Also posing a unique barrier is the corrosive steam oxygen environment.
- SOEC is versatile-can electrolyze either water (steam) or CO.
- They have selected reasonable electrode and electrolyte materials and are steadily increasing the scale of demonstration (stack size and number of stacks).
- Greater consideration to balance of plant issues should be given.
- Very sophisticated testing.
- Too bad heat balance was not investigated earlier to avoid need for CO_2 / H_2O mix.

- Project is too focused on building stacks for testing to meet milestones. These stacks often represent older technology versus the latest design. More effort is needed on cell research and development to solve problems at the component and sub-scale level, and not just full stacks.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- Seem to be meeting project milestones and learning as they progress.
- Delivered a four-stack module in March.
- Four stacks (60 cells each) have been delivered to INEL for evaluation. Progressing to this point is a major accomplishment.
- However, in a smaller demonstration with a 2-stack system it was noted that there was 50% performance degradation in first 600 hours. They ascribed this to failure of the manifold due to corrosion, which was constructed from 440 stainless steel. Perhaps more thought should have been given to selection of balance-of-plant materials/components prior to construction.
- Good progress, but tough to differentiate from SOFC progress.
- Building and testing at larger stacks and systems is progressing very well. Duration testing (for up to 2,000 hours) is also very encouraging. However, more effort must be placed on design and operation at conditions used in the process flow sheet, particularly steam-sweep for the oxygen electrode and pressurized operation.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- Good leveraging of SOFC technology in development of the SOEC.
- Good collaborations with national laboratories.
- Not obvious from poster/discussion.
- Collaboration between Ceramtec and INL is excellent. However, involvement with other solid oxide cell developers, such as the SECA program, should be pursued.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- Exercise production capacity, evaluate materials and process improvements, statistical performance distributions, extended lifetime testing, cell area scale up, stack size scale up and system BOP.
- Ceramatec with their partners will conduct an evaluation of the full ILS module.
- SOEC's could be a solution. Research plan seems solid.
- Project seems to focus on building more stacks at essentially the same design. More effort needs to be directed at cell scale-up, pressurized operation, operation at flow sheet conditions, and other advanced design options.

Strengths and weaknesses

Strengths
- Leverage of SOFC technology and potential for considerable scalability.
- High temperature steam electrolyzers have high efficiency and couple well to nuclear applications.
- Similarities to SOFC's.
- Good testing capabilities.
- Project has made great progress in building stacks and testing for extended periods.

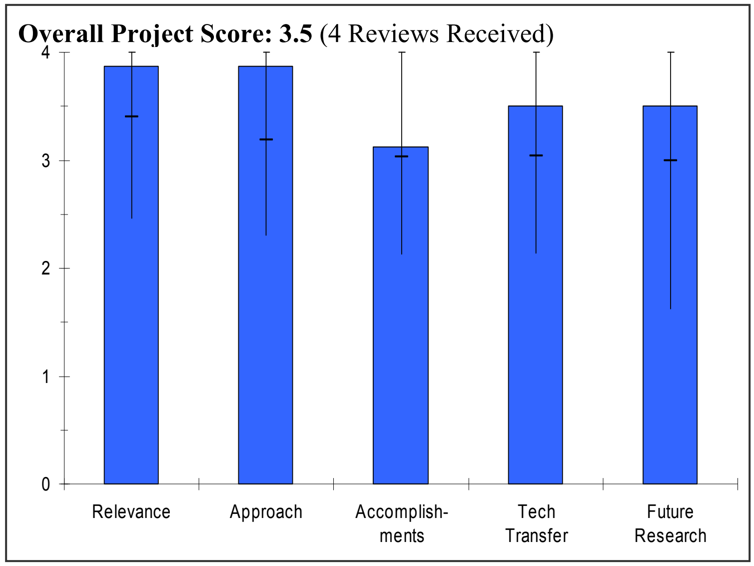
Weaknesses
- System operates at atmospheric pressure, so any compression will be a more significant cost than with other technologies. Presumably, the efficiency gains will more than offset these costs.

- Materials issues are the major problem with SOECs. Thermal cycling is an issue with regard to materials, especially interface integrity.
- Project needs more focus on fundamental and component development.

Specific recommendations and additions or deletions to the work scope

- Greater consultation on selection of balance of plant components is recommended.

Project # PDP-28: NHI Catalyst and Membrane Studies for Thermochemical Cycles at INL
Dan Ginosar; INL



Brief Summary of Project

The objectives of this project are to 1) develop enabling technologies for the sulfur-iodine (S-I) thermochemical cycle as a part of the Nuclear Hydrogen Initiative (NHI); 2) apply these technologies to the hybrid sulfur (HyS) cycle and to other non-sulfur based thermochemical cycles; and 3) have these technologies include effective catalysts for chemical conversion and membranes for chemical separations. These enabling technologies are needed to reduce the cost and increase the efficiency of the process.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.9** for its relevance to DOE objectives.

- The project supports overall DOE objectives by focusing on enabling technologies for DOE's prime candidate for thermochemical production of hydrogen.
- Research is focused on providing basic laboratory data for engineering modeling and design for integrated laboratory scale demonstration, which is necessary to meet DOE objectives.
- The sulfur/iodine cycle is still the front runner for thermo chemical water splitting using nuclear heat. Two barriers to commercialization of this cycle are the dewatering and decomposition of hydroiodic acid and the dewatering and decomposition of sulfuric acid. This project addresses both with good results.
- The project goals are critical to the Hydrogen Initiative and fully support DOE RD&D Objectives for thermochemical catalyst development for nuclear hydrogen production.
- This project is a critical part of the DOE-NE program to develop thermochemical cycles. The catalyst studies are particularly valuable. The membrane work may prove valuable as well, but it is less essential than the catalyst research.

Question 2: Approach to performing the research and development

This project was rated **3.9** on its approach.

- Membranes and catalysts were tested under expected process conditions and over a long enough period of time to detect degradation of performance.
- It is encouraging to see there are still new and innovative approached to be tried. This is a good piece of work.
- The project subtasks are well-focused on specific technical barriers and have been selected with respect to highest potential for impact.
- The project subtasks are well-balanced with respect to different technical barriers.
- The strategies for characterization of materials are well-described and robust.
- The strategy and rationale for resolution of key barriers for catalyst or membrane uniformity in composition, durability, and performance is logical and well-described.
- The contributions and responsibilities of collaborators and partners were clearly described.
- Both the catalyst and membrane research are sharply focused. The membrane work has less well-defined objectives which should be delineated..

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.1** based on accomplishments.

- Development of the project laboratory apparatus for testing in very harsh conditions required significant effort.
- Time constraints limited testing of additional membranes and more stable catalysts.
- Cause for deactivation of Pt catalyst has not been fully identified.
- The catalyst research does not appear to be complete enough to fully support the down select decision.
- The investigators have made significant progress. However, much work is still needed to address the durability of the sulfuric acid decomposition catalyst.
- The selection or derivation of specific milestones and performance indicators was difficult to discern; although, the investigators have clearly performed a great deal of work on testing of available catalysts.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.5** for technology transfer and collaboration.

- Closer collaboration with engineering team designing the ILS would provide feedback for further experimentation.
- This project at INL is well positioned to transfer technology developments to industry for scale-up and commercialization.
- There is a strong partnership and integration with other institutions and industrial enterprises.
- The complete characterization of various commercially-available catalyst materials will likely lead to opportunities for technology transfer and additional collaborations.
- Good collaboration between catalyst research and process developers, and national laboratories. Membrane research could use better interaction with potential system users.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.5** for proposed future work.

- The principle investigators have identified key research needs for these projects.
- Close collaboration with the ILS design team and performance feedback from that demonstration will facilitate optimization of the process.
- The investigators have outlines a good plan forward.
- The future research is well-described with respect to the desired target properties of the respective catalyst or membrane materials and their testing in an integrated lab scale stack.
- More specific performance milestones would help to guide both the catalyst and membrane research.

Strengths and weaknesses

Strengths
- The projects are very focused on providing appropriate experimental data to support design for the ILS project.
- The experiments were conducted at or near the expected conditions for the ILS.
- Innovative approaches to problem solving are strengths.
- The investigators demonstrate clear experimental design of each subtask, and have made significant progress in the project.
- Excellent technical approach and results.

Weaknesses
- The catalyst work timing does not fully support the ILS demonstration schedule.
- The lack of a system model or other means of predicting the impact of these novel modifications on the overall system efficiency is a weakness.

- Contingencies are not described and it is not clear how the investigators will actually use information from testing on actual decomposition in the down-select process among all available materials.
- The investigators are clearly expert in empirical testing; however, a more hypothesis-driven design of novel catalysts would be a useful addition to this project, either by inclusion of a new collaborator or utilization of in-house expertise.
- The selection of materials for testing seems somewhat ad-hoc and random, perhaps leading to decreased efficiency. Since no schedule or milestones were presented, it is difficult to discern how a more focused, strategic, and mechanism-driven approach might accelerate progress.

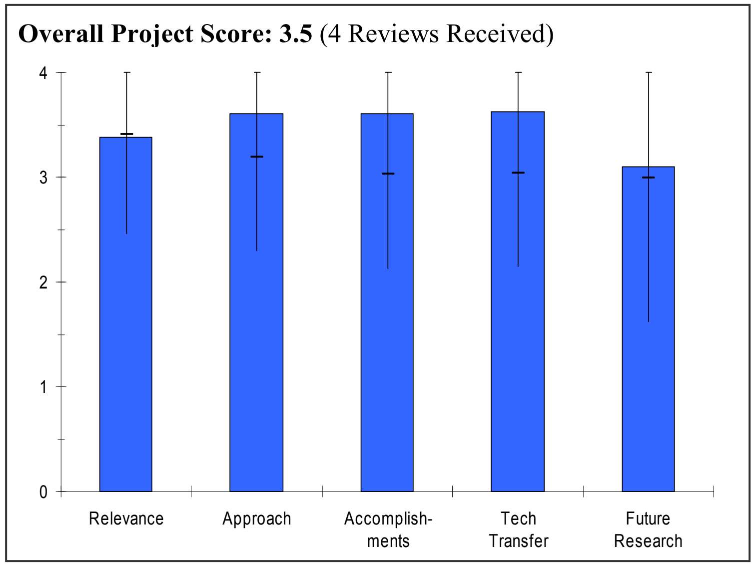
Specific recommendations and additions or deletions to the work scope

- The project scope should be expanded to include responding to feedback and providing support after the ILS demonstration starts. For example, experimental work may be needed to optimize the materials for sealing and supporting the separation membranes.
- Collaboration with General Atomics to do process modeling would accelerate process.
- More robust computational modeling or simulation might assist the investigators in choosing future commercially-available materials for testing.

Project # PDP-30: Materials Issues and Experiments for High Temperature Electrolysis and SO_3 Electrolysis
David Carter; ANL

Brief Summary of Project

The objectives of this project are to 1) determine causes of degradation in stack components from 25-cell stack tested for 1,000 hrs and 22-cell stack tested for 200 hrs and 2) develop oxygen and steam-hydrogen electrodes that show significantly improved area specific resistance and durability over state-of-the-art electrodes.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.4** for its relevance to DOE objectives.

- This project is well aligned with the DOE objectives. It is addressing important issues related to high temperature water electrolysis using solid ceramic electrochemical cells. As with all electrochemical devices of this nature, performance and durability are issues that must be addressed. This project is doing well to address these issues.
- The project goals are critical to the Hydrogen Initiative and fully support DOE RD&D objectives for thermochemical electrode development for nuclear hydrogen production
- Poster presents the work of two or three groups of people working fairly independently.
- The work appears to address corrosion issues relevant to the handling of steam/hydrogen and high pressure oxygen or air, as might be encountered in the operation of a nuclear-hydrogen production plant.
- Post-test evaluations for high temperature electrolysis (NIE) are an important part of that program. Work on SO_3 electrolysis needs a better defined focus and objectives.

Question 2: Approach to performing the research and development

This project was rated **3.6** on its approach.

- This project has brought to bear a sophisticated array of analytical equipment on the task of understanding the performance degradation mechanisms.
- The project subtasks are well-focused on specific technical barriers and have been selected with respect to highest potential for impact.
- The project subtasks are well-balanced with respect to different technical barriers.
- The strategies for synthesis and characterization of materials are well-described and robust.
- The strategy and rationale for resolution of key barriers for electrode uniformity in composition, durability, and performance is logical and well-described.
- The contributions and responsibilities of collaborators and partners were clearly described.
- The approach seems valid in exposing samples to prototypic conditions expected in a hydrogen production plant.
- Post-test examinations on the high temperature electrolysis stack were conducted thoroughly and with valuable results. However, the results need to be timelier and more closely linked with the construction of the next generation cells and stacks.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.6** based on accomplishments.

- The project made much progress on understanding the problems causing performance decay. Now that the problems have been identified, it should be easier to find solutions.
- The selection or derivation of specific milestones and performance indicators was difficult to discern; although, progress seems to be good for this recently-funded project.
- The two ANL tasks are apparently well advanced. The INL task is just getting underway.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.6** for technology transfer and collaboration.

- This project brings together two well respected national labs that are coordinating their work to address problems associated with high temperature water and sulfur trioxide electrolysis. Material components are being supplied by a manufacturer well positioned to take advantage of the results of the study.
- There is strong partnership and integration with other institutions and industrial enterprises.
- The synthesis of various experimental electrode materials and their complete characterization will likely lead to opportunities for tech transfer and additional collaborations.
- In the first two tasks there appears to be a good deal of collaboration between the national laboratories and the industrial partner.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.1** for proposed future work.

- Future plans are too generic. More specifics are needed regarding the approach and methodology to be used to select the materials to be studied.
- The future research is well-described with respect to the desired target properties of the respective electrode materials and their testing in an integrated lab scale stack.
- Recommend that the partners coordinate more closely.
- Future plans and objectives need better definition.

Strengths and weaknesses

Strengths
- Greatest strengths are the collaboration among partners and the capabilities of the analytical labs.
- The investigators demonstrate clear experimental design of each subtask, and have made significant progress in the project.
- This research may be able to identify the causes for the growth in cell resistance during operation.
- The second task may offer some understanding of the materials to be used in the balance of a hydrogen-production plant.
- The third task is an improvement of the standard sulfur-iodine cycle, but is somewhat unrelated to the other two tasks.
- Excellent technical work.

Weaknesses
- Having identified the problems, more focus is needed on the solutions.
- Contingencies are not described, and it is not clear how the investigators will actually use information from testing on actual decomposition to redirect synthetic efforts on other related electrode components.
- Need for closer coordination between the partners.
- Results need to be incorporated into the stack on a timelier basis.

Specific recommendations and additions or deletions to the work scope

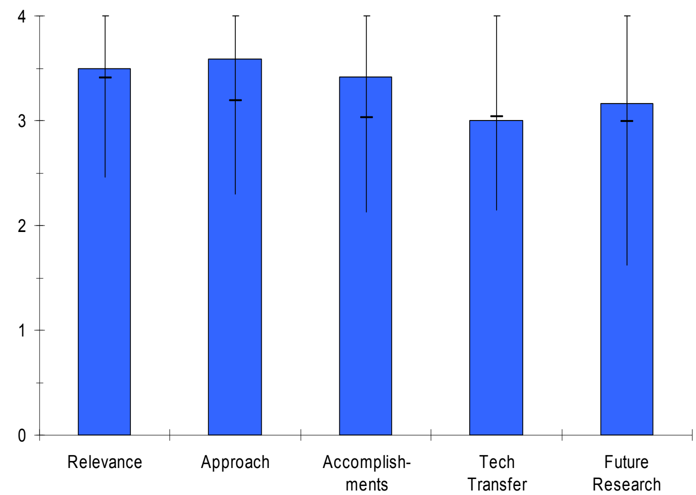
- Project scientists indicate that they would like to use XAFS as an analytical tool to sort out the chemistry. This seems reasonable to add to the project.
- Recommend that these three tasks not be grouped into one poster and thus into one review, since they deal quite different chemical environments.

Project # PDP-31: Corrosion Studies of Metallic Materials for Thermochemical Cycles
Bunsen Wong; General Atomics

Brief Summary of Project

The overall objective of this project is to develop heat exchanger construction materials for the hydrogen iodide (HI) decomposition process. The objective for 2004 to 2006 was the screening of materials candidates in HIx, HIx + H_3PO_4, concentrated H_3PO_4, and HI + I_2 +H_2 (gaseous). The objectives for 2006 to 2007 include: 1) stress corrosion and long-term testing of qualified candidates; 2) determining the effect of chemical contaminations on corrosion; and 3) testing of components with Ta cladding.

Overall Project Score: 3.4 (6 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

- The project is addressing an important problem in the Sulfur-Iodine Hydrogen cycle.
- Identification of appropriate materials for construction of heat exchangers and other process equipment is critical to the DOE objectives.
- Much needed research if nuclear Sulfur-Iodine thermochemical cycle is to be a component of the H_2 economy.
- Identification of corrosion resistant materials is critical to further development.
- Project supports DOE mission for nuclear hydrogen production by performing materials evaluation for selection of heat exchanger construction materials for use in the HI process. These are critical components.
- This work is essential to the development at the Sulfur-Iodine thermochemical cycle.

Question 2: Approach to performing the research and development

This project was rated **3.6** on its approach.

- The project approach is focused and well laid-out.
- The experiments and experimental apparatus are well designed.
- Tests of more complete systems (e.g., loops including valves, pumps, connectors at expected process pressures) are needed.
- Tests should include HI mixture contaminated with reaction products from the previous step (sulfuric acid and products).
- Excellent approach.
- Excellent simulation of actual operating conditions.
- Weld seam testing is excellent.
- Teflon components for processes at less than 200 degrees Celsius might be a viable, lower cost alternative.
- They are completing evaluation of materials through a balanced corrosion and mechanical properties testing. Long term testing is being accelerated through use of high pressure. Following this, scaled-up prototypes will be evaluated.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.4** based on accomplishments.

- Further testing of coated components, especially with respect to fabricated equipment (e.g., at welds) is needed.
- Good progress; excellent understanding and presentation of results.
- Will be very useful to the development of the Sulfur-Iodine cycles.
- Significant progress demonstrated. However, most of the accomplishments were specified for FY06 and FY05. No accomplishments specifically identified for FY07.
- They are 85% done, but will need additional funding next fiscal year. Most of the work has been tasked to UNLV. Appropriate materials have been selected for further test.
- Materials choices have been downselected to Ta alloy coatings.
- Project has been funded for three years; however, there is significant more work in materials evaluation to be conducted. Progression to scale up might have been expected at this point.
- More life-cycle testing, including cycling and potential upset conditions would be helpful.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- The project is collaborating with UNLV for mechanical testing and industrial support.
- They are collaborating with other researchers in industry for development of the complete system.
- It was not clear from the presentation how much the project has drawn on industry experience.
- General Atomics is the natural lead in this area; collaboration with UNLV should ensure that results become useful to others in the field.
- Degree of coordination between partners appeared to be fair.
- Only mechanical testing and analytical services were identified as UNLV contribution. Only one stress corrosion test result was reported.
- Only collaborations have been with UNLV.
- Project is closely linked with process developer.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.2** for proposed future work.

- The materials identification and testing program is winding down.
- The proposed longer-term testing of Ta-clad components is important.
- Project ends in September, so future work was not presented.
- Ideas for extending this work into demo units should have been proposed.
- Testing for FY06 - FY09 includes prototype testing, cost reduction studies and cross-contamination studies. All of these are important.
- In future research they will further test parts at elevated pressure.
- Ta coatings on copper and Teflon coated parts, to reduce cost, will be tested.

Strengths and weaknesses

Strengths
- The project is focused and well laid-out.
- The project has identified and tested suitable materials of construction.
- Systematic approach, proceeding from simple corrosion tests to component testing in process simulations is an effective way to screen materials.
- This was an area that needed research. Excellent approach.
- Large database of metal-corrosion test results from the 1970s at GA, Westinghouse and general literature, which was accessed.
- Balanced approach to materials testing and down-selection.

Weaknesses
- High pressure testing is needed.

- Future work is unclear. It is hoped that this effort, its results, and its follow-on don't get lost after project ends.
- The HIx section of the SI cycle has been flow sheeted in two ways: 1) reactive distillation and 2) extraction distillation. These two methods involve different process conditions and hence different materials may be needed.
- Not a lot of interactions outside UNLV.

Specific recommendations and additions or deletions to the work scope

- N/A

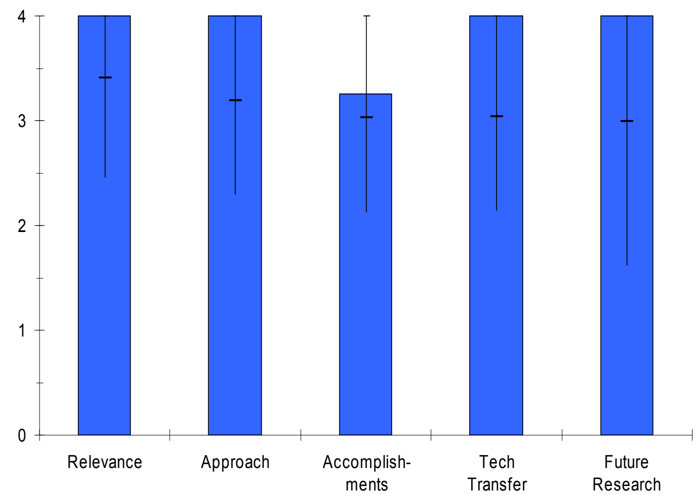
Project # PDP-32: Membrane Development for Hybrid Sulfur Electrolysis and Oxygen Separation
Mike Hickner; SNL

Brief Summary of Project

The Nuclear Hydrogen Initiative (NHI) is investigating thermochemical cycles as one of the promising methods for hydrogen production using Generation IV reactors. The sulfur-based cycles – Sulfur-Iodine and Hybrid Sulfur – are the focus of the current NHI research program. These cycles are the most technically developed of the more than 200 cycles reviewed and have the potential for high efficiencies. The ongoing work of this project includes:

- Ongoing high temperature permeation studies (Sandia National Laboratories);
- Continued structural elucidation;
- Determining the extent of corrosion during H_2SO_4 decomposition and possible mitigation steps;
- Continued membrane development (density, processing, scale-up);
- Testing on actual decomposition reactor.

Overall Project Score: 3.7 (2 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **4.0** for its relevance to DOE objectives.

- Needs addressed are critical to NHI program. Oxygen membrane will increase yields of SO_2 and O_2 for both sulfur cycles.
- Protein exchange membrane R&D, if successful, will eliminate or mitigate SO_2 carryover and allow successful deployment of hybrid sulfur cycle.
- The project goals are critical to the Hydrogen Initiative and fully support DOE RD&D Objectives for thermochemical process development for nuclear hydrogen production.

Question 2: Approach to performing the research and development

This project was rated **4.0** on its approach.

- Project started with the evaluation of known ceramic membranes for this application. This gives a good baseline.
- The project subtasks are well-focused on specific technical barriers and have been selected with respect to highest potential for impact.
- The project subtasks are well-balanced with respect to different technical barriers.
- The strategies for synthesis and characterization of materials are well-described and robust.
- The strategy and rationale for the mixed ionic-electronic conductor is good.
- The contributions and responsibilities of collaborators and partners were clearly described.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.3** based on accomplishments.

- Thermogravametric analysis data indicate promise, but also show more improvement is needed.

- Not clear what the O_2 permeation rate target is?
- Sulfonated Diels-Alder Poly(phenylene) (SDAPP) membrane performance is encouraging.
- The selection or derivation of specific milestones and performance indicators was difficult to discern, and relied substantially upon information provided by the presentation of the collaborator.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **4.0** for technology transfer and collaboration.

- There is no specific mention of collaborations.
- Found acknowledgement slide that lists many collaborations.
- There is strong partnership and integration with other institutions and industrial enterprises.
- The synthesis of various experimental membranes and their complete characterization will likely lead to opportunities for tech transfer and additional collaborations.

Question 5: Approach to and relevance of proposed future research

This project was rated **4.0** for proposed future work.

- The future research is well-described with respect to the desired target properties of the respective membranes.

Strengths and weaknesses

Strengths
- Extensive experience in ceramic and proton exchange membranes. Many contributors to project with 9 authors listed.
- The investigators demonstrate clear experimental design of each subtask, and have made significant progress in the project.

Weaknesses
- No overview slide and no approach slide were presented. Presenter told me that the project represented a $100K effort and had just started a short while ago.
- Contingencies are not described, and it is not clear how the investigators will actually use information from testing on actual decomposition to redirect synthetic efforts on other related membrane components.

Specific recommendations and additions or deletions to the work scope

- N/A

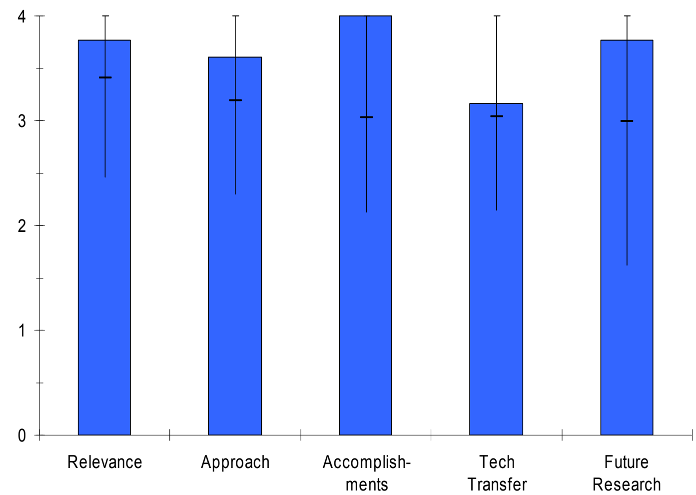
Project # PDP-33: Maximizing Light Utilization Efficiency and Hydrogen Production in Microalgal Cultures

Tasios Melis; UC Berkeley

<u>**Brief Summary of Project**</u>

The objective of this project is to minimize the chlorophyll antenna size of photosynthesis to maximize solar conversion efficiency in green algae. First, genes that regulate the Chl antenna size in the model green alga *Chlamydomonas reinhardtii* will be identified and characterized; then, these genes will be applied to other green algae, as needed. The approach is to interfere with the molecular mechanism for the regulation of the chlorophyll antenna size by employing DNA insertional mutagenesis and high-throughput screening to isolate tagged green algae with a smaller Chl antenna size.

Overall Project Score: 3.8 (3 Reviews Received)



<u>**Question 1: Relevance to overall DOE objectives**</u>

This project earned a score of **3.8** for its relevance to DOE objectives.

- Very relevant.
- The project goals are critical to the Hydrogen Initiative and fully support DOE RD&D Objectives for photobiological hydrogen production.
- Project supports MYPP long-range biological technology.
- Project supports a low greenhouse gas emission technology.
- Project represents a high risk, long-term technology, appropriate for DOE investment.

<u>**Question 2: Approach to performing the research and development**</u>

This project was rated **3.6** on its approach.

- They are attacking the main barriers to biological hydrogen production.
- The project subtasks are well-focused on specific technical barriers.
- The project subtasks are well-balanced with respect to different technical barriers.
- The approach has effectively addressed the barrier of photosystem inefficiency due to antenna size.

<u>**Question 3: Technical accomplishments and progress toward project and DOE goals**</u>

This project was rated **4.0** based on accomplishments.

- Impressive accomplishments with minimal funding, well done.
- The selection or derivation of specific milestones and performance indicators was well-described, with excellent progress towards specific performance parameters.
- The investigator has made good progress on the continued characterization of the Tla1 gene and its impact on regulation of Chl antenna size.
- The technical achievements are well-documented, including the identification of the specific defect in the Tla1 gene.
- Good progress – 2010 target already achieved with 2015 target coming within reach – despite significantly reduced DOE funding.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.2** for technology transfer and collaboration.

- There is not an industry partner, but then again there is not funding to support a partner.
- The potential for commercialization or tech transfer of the Tla1 gene is strong, with the investigators having filed a patent application on the use of this gene.
- The investigators demonstrate limited coordination and collaborations with external researchers.
- Since project focuses on answering limited scientific question with little engineering or immediate tech transition requirements – sole investigator is appropriate.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.8** for proposed future work.

- Good plans for the future research.
- The goal to clone the TlaX gene is logical, and should be doable given the investigator's past performance.
- The future research is narrowly-scoped, but has set clear goals with respect to measurement of antenna size.
- Proposed research has high probability of attaining target ahead of schedule.

Strengths and weaknesses

Strengths
- They have achieved a lot of results with minimal funding.
- Lots of publications and presenting at the Gordon Conference is impressive.
- The investigators demonstrate clear experimental design of each subtask, and have made significant progress in the project.
- The investigator is an expert in the biochemical and genetic study of *Chlamydomonas*.

Weaknesses
- Lack of funding.
- They should include calculations of the efficiency of incident light energy to hydrogen production.
- The project is extremely limited in scope, and therefore may not have significant impact on other research projects within the program.
- The potential for scale-up beyond small bench-top reactors is unclear.
- The investigator has not adequately addressed the question from the prior review—what is the proposed function of the Tla1 gene? The homology plot doesn't provide much information, and the fact that this gene is conserved across a diverse spectrum of species should allow the investigator to posit some hypotheses. This might lead to conducting a bioinformatics search for additional Tla1 homologs—or to devising some clues for function that might lead to a rational design or re-engineering of this protein.
- The investigator mentions the potential for transfer of this gene to other algal species. It is unclear whether this will work, since presumably any algal homologs would be revealed in the initial bioinformatics screen.

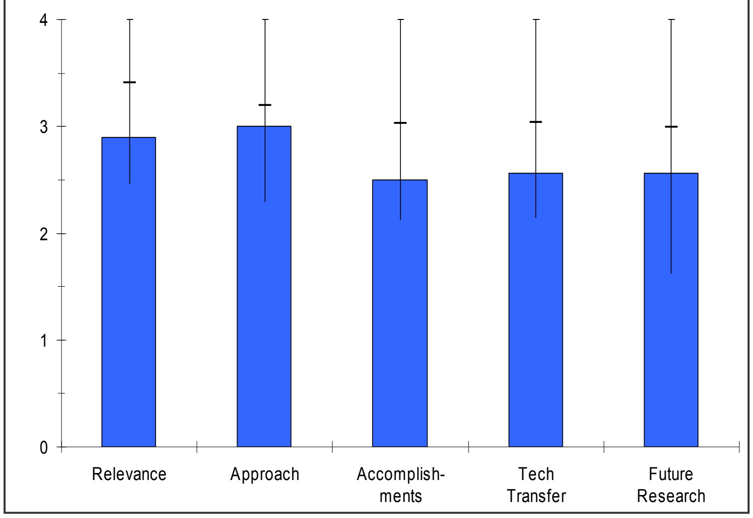
Specific recommendations and additions or deletions to the work scope

- Scope (and funding) should be enlarged to include duration of production and oxygen tolerance.

Project # PDP-36: Photoelectrochemical Generation of Hydrogen Using Sonicated Hybrid Titania Nanotube Arrays
Mano Misra; U of Nev. Reno

Brief Summary of Project

Overall Project Score: 2.7 (5 Reviews Received)



The overall objective of this project is to develop a high-efficiency photoelectrochemical cell using titanium dioxide nanotubular photo-anode and cathode for hydrogen generation by water splitting. The objectives for FY 2006-2007 are to 1) develop a new anodization technique to synthesize high-quality and robust TiO_2 nanotubes with a wide range of nanotube architectures; 2) develop single-step low band gap TiO_2 nanotubes by modifying synthesis parameters; and 3) develop a kinetics and formation mechanism of the titanium dioxide nanotubes under different synthesis conditions. For FY 2007-2008, the objectives are to improve efficiency by mixed oxide and organic-inorganic semiconductor photo-anodes; develop density functional theory to identify and modify the electronic properties of nanotubes; develop a combinatorial approach to synthesize hybrid photo-anodes having multiple hetero-atoms incorporation in a single photo-anode; and develop new TiO_2-based cathodes to increase the efficiency of the photoelectrochemical cell.

Question 1: Relevance to overall DOE objectives

This project earned a score of **2.9** for its relevance to DOE objectives.

- Most project aspects align with the Hydrogen Initiative.
- TiO_2 has been studied extensively for PEC water splitting applications, and it's severe limitations in terms of bandgap, absorption and electron transport are well established; this is another case of starting over with a 'comfortable' material. While at least making some case for improvements to transport (through nanotubes) and bandgap (through "carbon" modification), the case was not compelling in this presentation.
- Considering the external bias requirements for effective photocurrent levels in this TiO_2 work, and the lack of a clear pathway for achieving the longer-term DOE photocurrent and STH efficiency goals with this material system, this work did not adequately address the DOE RD&D objectives for unassisted PEC solar water splitting.
- There may be conceivable pathways toward DOE RD&D objectives with substantial breakthroughs in TiO_2modification in conjunction with multi-junction device configurations; however these pathways were not apparent in this presentation.
- Project supports MYPP for photoelectrochemical production of hydrogen.
- Difficult to differentiate from conventional TiO_2, which is known not to work.
- Not clear how/why nanotubes are an improvement.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- Step-wise logical approach.
- Does not appear overly ambitious considering the group and funding level.
- Durability testing and cost estimation is lacking in approach.

- The approach of TiO_2 nanotubes for enhancing charge transport and surface area is interesting, but does not address fundamental absorption limitations of the material.
- The approach of carbon mondified TiO_2 for bandgap reduction has received much press in recent years, but the beneficial effects in visible light absorption have been generally overstated in literature, and also in this presentation. The bandgap limitations in this material class generally represent a show-stopper, and until there is clear evidence that radical band modifications are possible without complete destruction of optoelectronic properties, no amount of "nano-structuring" will matter.
- The approach for synthesizing TiO_2 nanotubes presented appears to be very effective.
- The approach of employing "off the shelf" materials modeling software for atomistic modeling and DFT is good, producing pretty pictures and graphs. The model results presented however appear somewhat 'first order', and will need some careful refinement for achieving realistic representation of the TiO_2 material system. For example, the direct bandgap indicated in the DFT calculations were particularly surprising – although this may be possible in novel atomistic structures of TiO_2 – it isn't commonly seen, and it wasn't supported in the presented data (which clearly indicated indirect bandgap). More application of the theory to validate the bandgap effects (for example of "carbon-modification") should have been a more significant part of the approach here – this would have required a greater allocation of the program's substantial resources in this challenging theoretical activity as well as a much greater reliance on external expertise, but it would be essential in addressing the main issue limiting TiO_2 in PEC applications.
- The approach of Pt Nanoparticles on TiO_2 nanotubes as an effective counterelectrode may be interesting in other higher-current density applications, but may be overkill in the solar conversion applications in which current densities remain low. Non-noble catalysts can be perfectly adequate in such applications.
- It was good to see some work on 'scaling up' the electrodes, however this is somewhat premature since the current material system is not functional for direct solar water splitting.
- Generally good (in discovery phase).
- Have identified potential roadblocks, so next year is crucial.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.5** based on accomplishments.

- Modest progress considering the amount of funding.
- Unclear why doing the carbon doping.
- Accomplishments in terms of TiO_2 nanotube synthesis were impressive.
- Accomplishments in atomic modeling and DFT calculations were interesting, although in need of further refinement.
- Reported accomplishments in terms of carbon-doping of the TiO_2 nanorods were not clearly supported either in XPS or photocurrent data.
- The implied bandgap reduction in "carbon doped TiO_2" was not sufficiently supported experimentally or theoretically; In fact, the IPCE measurements shown clearly reflect a material with some UV sensitivity, but still little visible sensitivity.
- Most of the photocurrent data presented was based on very questionable application light sources – a common error in PEC measurements. It is apparent that the light source utilized in the photocurrent measurements substantially over-compensates in the UV, which can make wide bandgap materials (which are unacceptable for PEC water splitting) look reasonably photoactive. The use of carefully calibrated light sources validated by outdoor sun measurements is critical to PEC research, especially in the evaluation of wide bandgap materials; considering the resources of this program, there is no reason for not implementing such fundamental experimental procedures.
- The conclusion that this work represents a "highly efficient photoelectrochemical cell for solar hydrogen generation by water splitting" is misleading; the need to operate under external bias and the application of illumination not representative of the solar spectrum contradicts this conclusion. That being said, it was at least encouraging to see any photocurrents in the mA/cm^2 range in TiO_2 material; the important issues in bandgap modification for non-UV absorption need to be more rigorously addressed in this work, with better theoretical and characterization efforts, and in conjunction with more experienced research partners.
- Concerned that investigator is 30% complete at this point in project.
- Reasonable progress in one year.
- Still skeptical regarding ultimate success.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.6** for technology transfer and collaboration.

- Unclear how group is working together.
- There was no clear indication of collaboration with any of the purported "partners"; help from other stated collaborators would prevent the types of photoelectrochemical measurement errors demonstrated.
- In light of the significant financial resources involved, collaboration with more experienced partners would have contributed enormously to the quality of the work.
- The concept for bandgap reduction in carbon-modified TiO_2 was clearly based on the work published by Dr. Khan at Duquesne University; this should have been cited, and collaboration with Dr. Khan should have been considered.
- TiO_2 for solar water splitting has been studied extensively over the years, and TiO_2 nanotubes have been explored. The fundamental limitations of absorption and carrier collection are still critical ones and still unsolved; if this work wants to work toward the significant breakthroughs that would be needed, a seriously expanded collaboration involving more experienced partners would be needed.
- Broad partnership: academic, national lab and industrial partners, including an international partner.
- Not clear how collaboration is carried out.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.6** for proposed future work.

- Plans may lead to improvements, but unambitious for amount of funding.
- The proposed future work was a smorgasbord of popular ideas and buzzwords taken from TiO_2 literature.
- Some of the ideas were of interested, but not relevant until there is solid justification that efficient unbiased solar water splitting is achievable in a TiO_2 material system.
- Significant future remains in reducing TiO_2 bandgap, increasing the portion of the spectrum that the material can harvest, while reducing cost: uncertain that remaining funding is sufficient to overcome challenges.
- Need to increase their absorption efficiency.
- Need to show election mobility for long tubes.

Strengths and weaknesses

Strengths
- Lots of publications.
- Good modeling.
- Synthesis of TiO_2 nanotubes.
- Use of atomicistic modeling and DFT.
- Demonstration of photocurrents in the mA/cm^2 range.
- Novel idea.
- Well carried out.

Weaknesses
- Unambitious goals.
- Many people have made TiO_2 nano tubes.
- Misleading photoelectrochemical results based on improper utilization of light sources.
- Inadequate collaboration with more experienced technical partners.
- Does not identify a clear pathway toward efficient unbiased solar water splitting based on TiO_2 material.
- Inadequate utilization of program resources in appropriate theoretical and characterization activities for solving the main technical barriers.
- Perhaps relying on "nano-enabled miracle"; i.e., nano-solution that doesn't exist.

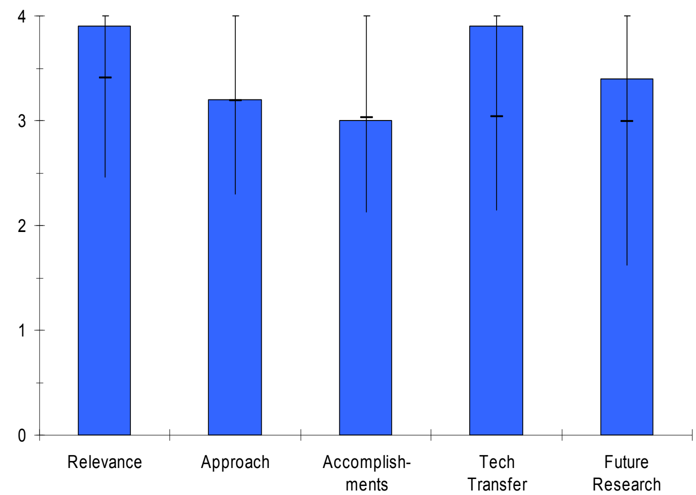
Specific recommendations and additions or deletions to the work scope

- Should add durability study.
- Should add cost analysis.
- The resources allocated to this work, if applied correctly, should be sufficient to identify once and for all whether TiO_2 has any chance of success in an efficient unbiased solar water splitting system. Expanded collaboration with other experienced research partners in materials science and photoelectrochemistry would be a necessary addition for this.
- There needs to be more emphasis on the fundamental theoretical and experimental approaches to defining the limits of bandgap modification and the implication on the ultimate efficiency of solar water splitting based on a TiO_2 system
- Less emphasis on the novel counterelectrode structure.

Project # PDP-37: Photoelectrochemical Hydrogen Production: UNLV-SHGR Program Subtask
Eric Miller; UNLV

Brief Summary of Project

Overall Project Score: 3.4 (5 Reviews Received)



The primary objective of this project is to assist the DOE in the development of hydrogen production technology utilizing solar energy to photoelectrochemically split water. The primary focus is on low-cost thin film materials (such as metal oxides) and novel multi-junction thin film devices (such as the UH-Hybrid Photoelectrode-HPE). The specific UNLV-SHRG photo-electrochemical (PEC) project goals are to 1) identify and develop new PEC film materials compatible with high-efficiency, low-cost H_2 production devices; 2) demonstrate a functional multi-junction device incorporating best-available PEC film materials; 3) develop avenues, integrating new theoretical, synthesis and analytical techniques, for optimizing future PEC materials and devices; and 4) explore avenues toward manufacture-scaled devices and systems.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.9** for its relevance to DOE objectives.

- This is relevant to the Hydrogen Program.
- Project is working to provide a feasible path to the DOE targets.
- Large collaborative effort appears to be an efficient approach to working towards DOE PEC cost and efficiency targets.
- Economical photoelectrochemical production of hydrogen is a viable and important long-range DOE objective.
- Despite decades of research, significant materials issues remain to be resolved; hopefully, a teaming arrangement will be of great aid in focusing individual researcher efforts to accomplish goals of efficiency, cost and materials stability.
- Great cross-university/industry/national lab collaboration covering multiple topics.

Question 2: Approach to performing the research and development

This project was rated **3.2** on its approach.

- Good combination of modeling and experimental work.
- Good team and collaboration.
- Focusing on the correct problem (materials).
- It took too long to arrive at the team approach.
- The feedback loop is beneficial in developing the theory and characterization of materials.
- Because each material presents different challenges and is being evaluated on progress toward overcoming those challenges, the project team needs to ensure that they are being evaluated against the same overall criteria.
- Initial screening via combinatorial modeling allows for quicker focus on most promising film compositions.
- Broad based participants allow faster synthesis, characterization and screening.
- Feedback loop good for quick incorporation of new learnings into subsequent experimentation.
- Work with NREL provides necessary integration into larger PEC system design.
- Though a teaming arrangement, this project is simultaneously pursuing several (5) different classes of materials.

- The benefit of this approach will be the development of theoretical tools that will help all participants and periodic (quarterly) group feedback can accelerate attainment of R&D goals.
- The team on this project should further develop effective measures to down select materials to focus on the most promising material(s).
- Multijunction, tandem approach for catching large amount of the solar spectrum appears to be a reasonable approach to improve device efficiency.
- Theory-synthesis-characterization-feedback is a logical approach.
- Good team, but perhaps too much "shotgun" approach.
- Could use more focus.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- Minimal progress with the team they have and the time spent.
- The project has made good progress in the past year.
- It is unclear how much DOE funding will be needed to continue or complete the planned work.
- Photocurrent milestones met for several PEC films.
- Highest efficiency achieved is 3.1%. This is much better than decades ago (1%?) but still very far from DOE's goal of 10-15%.
- Combinatorial synthesis approach is useful.
- Understanding of the effect of additions (e.g., nitrogen in tungsten oxide) is useful new knowledge.
- Materials-specific information gained for all 5 classes- a good body of data has been generated and is being applied to improve materials and structures.
- Good work thus far.
- Too much to present in one poster at any depth.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.9** for technology transfer and collaboration.

- With the new teaming plan they are now starting to share their results.
- Excellent collaboration - this project really leverages teams from all types of organizations.
- Large ongoing collaboration that meets quarterly for information sharing.
- One of the strongest aspects of this project is the number of partners involved.
- Absolutely outstanding that so many people can work together effectively.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.4** for proposed future work.

- There is no clear path to achieve the ultimate goals.
- They have set up a good plan on how to accomplish interaction and coordination.
- Need hard go/no go decision point to down-select materials.
- Covering a variety of technology options each with clear targets.
- Down-select of materials has been started. P.I.s should make sure that they accomplish this so more resources can be directed towards the most promising materials, structures, and fabrication procedures.

Strengths and weaknesses

Strengths
- Combinatorial approach.
- Strong group that is starting to act as a team.
- All of the available expertise.

- Team feedback approach and sharing of theory tools and cluster tools, and other insights. Took 2 years to get everyone together.
- Wide talent base.

Weaknesses
- Slow progress for 3 years of development.
- They have not used the combinatorial approach to its potential.
- No funding for 2007- did not request an explanation.
- Unclear how momentum continues without government funding.
- People have spent decades researching photoelectrochemical devices. Time will tell but there is the possibility that these (or any) investigators may only be able to make marginal improvements. Should have a number of go/no go decision points in the coming years.
- Too much independent work.
- Lacks focus.

Specific recommendations and additions or deletions to the work scope

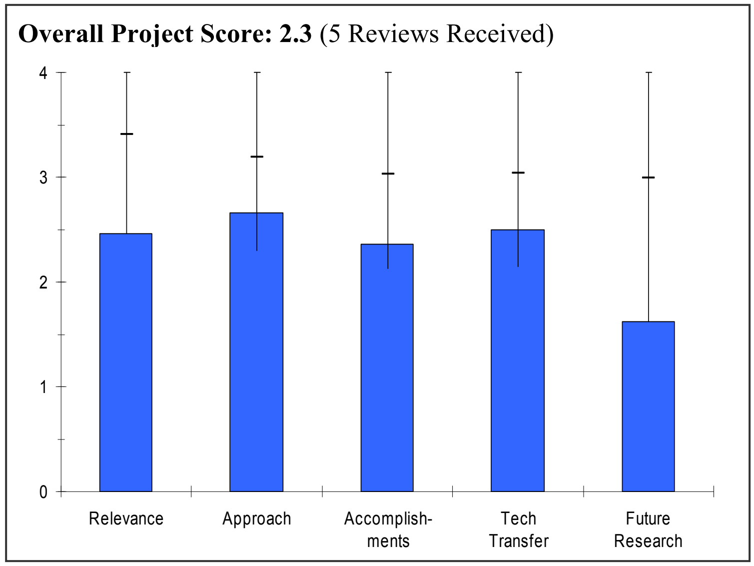
- Develop a path to achieve their ultimate goals. There is no path beyond discovery.
- Develop go/no go decision points for each class of materials.

Project # PDP-40: Adapting Planar Solid Oxide Fuel Cells for Distributed Power Generation

Andres Marquez; Ohio University

Brief Summary of Project

The objective of this project is to quantify impacts of synthesis gas composition on performance of a commercial planar solid oxide fuel cell system (cell and stack) that includes: 1) H_2S content; 2) CO/H_2 ration and energy content of gas; 3) particulate; and 4) metal content. The objective also includes the demonstration of long-term operation of planar solid oxide fuel cells (pSOFCs) using actual solid fuel-derived synthesis gas. pSOFC area specific resistance (ASR) was measured by completing V-I scans; the ASR histories were plotted and studied. Additionally, voltage (power) performance over time was monitored and studied.



Question 1: Relevance to overall DOE objectives

This project earned a score of **2.5** for its relevance to DOE objectives.

- This is focused on electrical production not hydrogen production. It is not directly relevant to the President's Hydrogen Fuel Initiative.
- This project seems to be aligned with SECA and should be done in that program.
- The use of syngas as a fuel for solid oxide fuel cells (SOFC) is an objective of the DOE Distributed Generation program.
- The project addresses improved tolerance to CO, H_2S, and other contaminants in syngas.
- Integration of SOFC and coal gasification could be a very likely scenario for stationary power generation.
- To further assess the relevance, it will be useful to look at the economic analysis of such an integration approach.
- Project focusing on effect of contaminants on solid oxide fuel cell performance. Similar work being conducted through the SECA program. Presumably, PI will communicate results to the solid oxide community at large.
- Solid oxide fuel cells have the highest efficiencies of all fuel cells; however, there are major materials issues to be resolved including poisoning, sealing, thermal cycling, etc. The proof will be the development of stacks (which this project is not doing) and long-term evaluation.
- The work appears to be competent, but the task does not appear directed toward the production or delivery of hydrogen. Appears that the managers of this review meeting have either placed this task in the wrong group, or that the task does not fit comfortably into the existing groups.
- Why has the funding been zero for the last two years?
- Appears to be answering a question of relevance to the FE or SECA programs?
- Work may have much higher relevance if SOFCs are used for the production of synthesis gas by stack gases containing H_2S.

Question 2: Approach to performing the research and development

This project was rated **2.7** on its approach.

- The integrated energy vision is not realistic since they are performing a water gas shift reaction prior to the Fischer Tropsch (FT) reactor (this changes the hydrogen to carbon monoxide ratio to a less desirable ratio). They are removing the carbon dioxide using a room temperature approach and then having to heat the gases back up, a method to remove carbon monoxide prior to the PEMFC is not included, and desulfurization was not included. The process produces a lower value commodity (electricity) at the expense of a higher value commodity (FT fuel).

- They did not properly identify the barriers to be addressed, or how their work is pertinent.
- The approach is not very original.
- The approach to quantifying and identifying the effect of contaminants in SOFC performance is good.
- The project does not sufficiently address mitigation of the contaminants or modifications to SOFC design to minimize the impact of the contaminants.
- The project scope is limited to the SOFC degradation mechanisms.
- One should not only look at the impurity impact, but also other aspects of coal gasification and SOFC integration. What are the critical barriers? The most critical ones should be addressed first.
- Generally the approach is narrowly focused. The right framework is to start with a broad set of challenges and down-select the showstoppers.
- PI is evaluating the effect of several contaminants (H_2S, HCl, AsH_3) on button cell performance.
- Button cells were provided by commercial vendor. No new materials were investigated in this work.
- Within the limitations on relevance to hydrogen production and delivery noted above, the approach is competent and effective.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.4** based on accomplishments.

- It appears that no improvements to the system were made.
- The project has identified the contaminants in syngas that are deleterious to the SOFC. The effect of trace levels of contaminants on SOFC degradation has been quantified.
- The project has not identified mitigation strategies.
- The progress is extremely slow and very little was accomplished for the time that has elapsed.
- Due to switching of SOFC partners a lot of work needs to be redone and very little time left for the project completion.
- Technically the only nugget that stands out is a sulfur tolerant anode catalyst.
- Low level of progress for funding level of project.
- Very low power density (less than 200 mW/cm^2) for button cells makes the design/materials not suitable for commercialization.
- PI has not made apparent significant progress toward most important DOE goals (40,000 hrs durability and $1000/kWe).
- Severe cell degradation noted in this work.
- Progress seems to be good for a three-year task. However, the task has been going for five years and has not received any funding during the last two years. Shouldn't it be completed?

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.5** for technology transfer and collaboration.

- How the team interacts is not clear.
- No papers or presentations were reported.
- The project is testing a commercial SOFC and is interacting with the manufacturer.
- The project is also working with other universities.
- Poor collaboration/selection of partners – switching the cell provider at such a late stage has caused significant perturbation to the project deliverables.
- Unclear how/who this technology will be transferred to. Button cell is a very early stage platform. Scale-up challenges are significant going from button cell to a representative stack scale.
- Several partners, but roles are uncertain.
- There appears to be a good deal of collaboration within the state of Ohio and some funding from state agencies.

Question 5: Approach to and relevance of proposed future research

This project was rated **1.6** for proposed future work.

- No future plans were reported in the poster.
- The project is winding down.
- Proposed future work is longer-term testing.
- The presentation did not adequately address future work beyond testing.
- Proposed future research is inadequate to meet the said objectives of the project. This is mostly due to rework resulting from the shift in the cell partner.
- PI has collected data on effect of contaminants on cell performance, but it is uncertain of how this will be used to improve materials performance.
- Future work not presented.
- It appears that the project is ending or has ended some time ago. There are no suggestions or recommendations for future work by others taking on a similar project.

Strengths and weaknesses

Strengths
- Use of actual gas from coal gasification as the feed is useful.
- The project has made progress in identifying contaminant concerns in SOFCs.
- Good relevance to DOE's technical and portfolio goals.
- This work has identified what level of contaminants can be allowed beyond which unacceptable cell performance occurs.
- The causes of the performance loss have been identified.

Weaknesses
- The project focuses on SOFC work which should be part of the SECA program.
- There is nothing reported for future work.
- The scope of the work is limited.
- The project does not address improvements to SOFC technology. Some of this is being addressed in a companion project.
- Poor teamwork/partner strategy.
- Extremely slow progress - possibly due to lack of appropriate personnel on the project team.
- No new materials development.
- Little explanation of how the information gained in the task should be used in the fabrication of future cells.

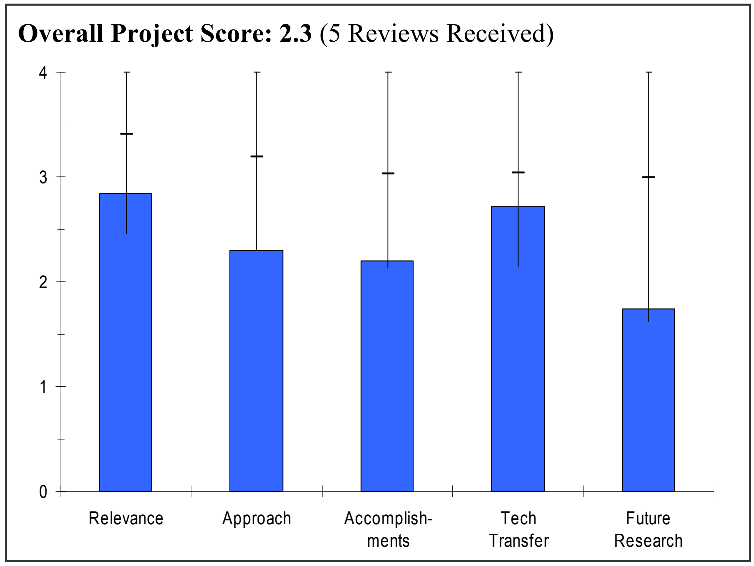
Specific recommendations and additions or deletions to the work scope

- The project should be transferred to SECA or the fuel cell group.
- Their progress needs to be compared to DOE goals.
- Future work needs to be planned.
- They need to do some simple flow sheet modeling using ChemCad or Aspen to look at the "integrated concept".
- Given the progress, the said scope is adequate. Further addition will further delay the project. Any deletion of scope might significantly hamper the usefulness of the project.
- Include recommendation for future research in any final report from this project.

Project # PDP-42: Ohio Distributed Hydrogen Project
David Bayless; Ohio University

Brief Summary of Project

The objective of this project is to develop technology to aid in creation of a viable "distributed energy" system that 1) provides electricity from stationary solid oxide fuel cells; 2) provides useful waste heat from the fuel cells for other unit operations; and 3) provides usable hydrogen from the synthesis gas. The objective also includes the integration of combined heat and power into distributed H_2 production.



Question 1: Relevance to overall DOE objectives

This project earned a score of **2.8** for its relevance to DOE objectives.

- The main focus of the project is not hydrogen production, but hydrogen production is part of it.
- The project is developing technology to improve integration of a distributed energy system.
- The program aligns with the DOE distributed energy goals.
- Integration of SOFC and gasification could be a very likely scenario for stationary power generation.
- The overall "integrated energy vision" as highlighted in the project is good. But still unclear as to how the project will address the critical barriers in realizing the vision. Too broad a scope for the project.
- This project is focused on the development of solid oxide fuel cell technology for distributed energy production, and CHP applications. Integration of CHP into hydrogen production is a key element and important first step in development of the hydrogen economy. CHP applications have high efficiency.
- Project is also evaluating ceramic membranes for hydrogen separation for pure hydrogen fuel stream.
- This project is part of a novel combination of coal gasification and the growth of algae for the production of hydrogen.
- It appears to reflect some 'out of the box' thinking and thus cannot be comfortably placed in a particular category.

Question 2: Approach to performing the research and development

This project was rated **2.3** on its approach.

- The integrated energy vision is not realistic since they are performing a water gas shift reaction prior to the Fischer Tropsch (FT) reactor (this changes the hydrogen to carbon monoxide ratio to a less desirable ratio), they are removing the carbon dioxide using a room temperature approach and then having to heat the gases back up, a method to remove carbon monoxide prior to the PEMFC is not included, and desulfurization was not included. The process produces a lower value commodity (electricity) at the expense of a higher value commodity (FT fuel).
- When reporting data for the sulfur tolerance, the operating temperature, anode gas composition and fuel utilization should be reported.
- The electrolysis and separation approach is interesting.
- The fuel cell work is exactly the same as project PDP-40.
- The project is addressing three distinct areas: improving sulfur tolerance of SOFC anodes improving ceramic membranes for H_2 separation and optimizing H_2 production in the gasifier.
- The project effort is too divided among the three aspects. The project is not integrating the three aspects.

- The approach is narrowly focused, given the scope of the project. Most of the work is on SOFC development, with little emphasis on Fisher Tropsch synthesis and other separation steps (e.g., CO/H_2 and H_2).
- First step shall be to determine the economics of the grand scheme and then down-select the right element to focus on. Does it make sense for this whole cycle? What is the cost of (PEM grade) hydrogen from this scheme? What is the overall efficiency? All these questions need to be answered first.
- Project is developing sulfur tolerant anodes, a critical issue for solid oxide fuel cells.
- CHP configuration is being evaluated for highest efficiency.
- Pressure effects, H_2S effects, membrane flux, fluidized bed gas yields all preliminarily evaluated.
- It is felt that too many topics are being pursued in this project and that this will be problematic for making significant progress in any one particular area.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.2** based on accomplishments.

- There has not been a significant progress toward the stated objectives.
- The project has identified an improved SOFC anode and conducted short-term testing.
- The progress in ceramic membranes is hard to judge, as state-of-the-art membrane data were not provided.
- The technical merits (and parameters) of the MEIC and H_2 separation membrane work were unclear and should be described in further detail.
- Technically, the only nugget that stands out is a sulfur tolerant anode catalyst, which is shared with PDP-40.
- Quantification of targets for each stage of the project will help in assessing the accomplishments.
- No data shown for different electrode materials.
- Button cells provided by external vendor so the researchers have not performed valuable materials research.
- Pressure effects, H_2S effects, membrane flux, fluidized bed gas yields all preliminarily evaluated. A mix of a "bunch of stuff." It is unclear how this all adds up to meet project goals.
- I don't see any energy balance to the various processes, including the electrolytic step.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.7** for technology transfer and collaboration.

- The coordination is unclear.
- There were no papers or presentations reported.
- The project is working with two other universities.
- Good teamwork/collaboration between the partners – the work on H_2 separation needs to be discussed in further detail.
- Need to lay-out a plan for future technology transfer.
- Several partners, but roles are uncertain.
- There must be close collaboration with their industrial and state government partners. Doesn't appear that DOE has been providing funding recently.

Question 5: Approach to and relevance of proposed future research

This project was rated **1.7** for proposed future work.

- No future work was plans reported.
- The presentation did not address proposed future work.
- The project does not appear to have any go / no go or down selection criteria.

- Proposed future research is inadequate to meet the said objectives of the project. This is mostly due to the broad scope of the project.
- Quantification of individual subtask targets will be useful in assessing the merits of proposed future work.
- No future research discussed.
- No real suggestion of future research. Appears that the project is barely existing on outside support.

Strengths and weaknesses

Strengths
- They are examining sulfur tolerance.
- They are looking at some high temperature ceramic electrolysis and separation.
- Good relevance to DOE's technical and portfolio goals.
- Novel approach.

Weaknesses
- The integrated energy vision is unrealistic. The water gas shift reactor is in the wrong place.
- The models need validation.
- The electrolysis work is not original.
- The project is not integrated.
- The project effort is divided and lacks focus.
- Broad scope of the project. Would help to descope some of the activities.
- Very low power density for button cells makes the materials unattractive to scale up to a stack and commercialization.
- Project is pursuing several lines of research-solid oxide fuel cells, CHP application, and ceramic membranes for hydrogen separation. Should focus on only one line for greater benefit to DOE goals.
- Very inconsistent funding and little vision of future directions.

Specific recommendations and additions or deletions to the work scope

- The fuel cell work should be removed.
- The project should focus on only one or two areas.
- The project should be descoped to improve its efficacy. Focus should be entirely directed first towards the economic assessment and then down-selection of critical barriers to be addressed. This will help in narrowing and downselecting the right focus.
- Progress in this project has been slow and it is recommended that the project should be discontinued.
- The project should either be properly funded then reviewed, or, if it is not funded, it shouldn't be reviewed.

2007
Hydrogen Storage
Summary of Annual Merit Review Hydrogen Storage Subprogram

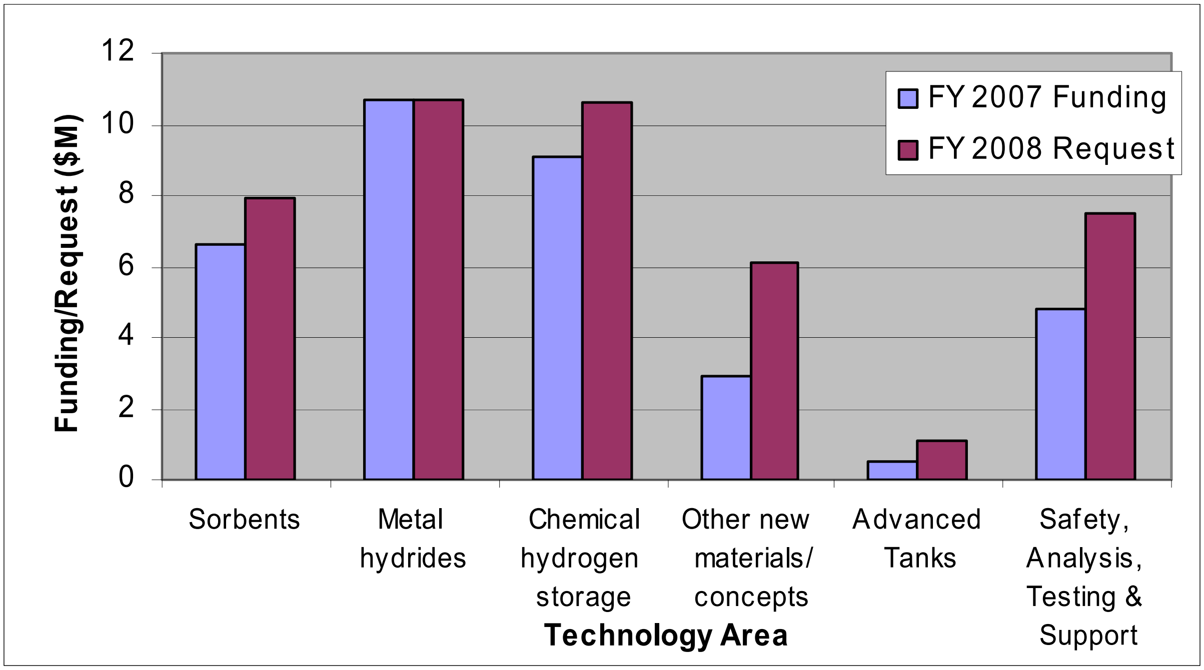
Summary of Reviewer Comments on Hydrogen Storage Subprogram:

Reviewers stated that the Hydrogen Storage subprogram was well focused with a robust R&D portfolio, clear ties to technical targets and well managed at all levels, both strategically and at the project level. Reviewer comments indicated that management of such a large and comprehensive effort with more than 80 projects requires coordination and sufficient program management resources. It was also noted that the Storage subprogram coordinates extensively with international activities as well as with the FreedomCAR and Fuel Partnership Technical Team and DOE's Office of Science. Reviewers stated that "the Center of Excellence approach on each main topic is an excellent and efficient way to pool resources for the R&D and provide clear focus to the participants." Of particular interest was the new Engineering Center of Excellence (CoE), which will help address systems issues often neglected by the other centers, and provide insight on the overall efficiency, cost, thermal management strategies, and the impact on system design and hydrogen delivery infrastructure.

Reviewer recommendations to the program included maintaining the processes to add new center and independent projects to ensure flexibility and agility. For the CoEs, it is important to continue to ensure transparency on the methods of operation and management (e.g. structure, decision process, communication flow & synergy among the sub-program areas, IP management). It is critical that the CoEs have mechanisms to share experiences and lessons learned particularly on cross-cutting issues. Engineering issues and tank system design could be further emphasized and the researchers should be encouraged to address them earlier on in the program. DOE was encouraged to continue reminding researchers that they must address system targets and not focus only on gravimetric capacities of materials. For example, the program should start emphasizing safety and toxicity issues for the benefit of all researchers as well as the role of such issues in the down-selection process. More emphasis was recommended on infrastructure issues and how various storage alternatives affect the well-to-wheels energy efficiency. Reviewers also recommended that the program start a review of the portfolio and assess the progress to date. Finally the CoEs should be encouraged to collaborate with each other as well as with independent projects and groups outside the DOE portfolio as appropriate.

Hydrogen Storage Funding by Technology:

The funding portfolio for hydrogen storage addresses primarily long-term materials R&D to meet 2010 and eventually 2015 targets for on-board applications. The requested EERE FY2008 funding profile, which includes the CoEs and independent projects, continues to address the National Academies' and FreedomCAR and Fuel Partnership's recommendations. Plans for FY 2008 (subject to congressional appropriations) include initiating a new Center of Excellence on applied engineering R&D to address system issues, as recommended by reviewers. The storage subprogram also plans to continue its annual solicitation to allow flexibility in eliciting new concepts and approaches that may not be in the current portfolio. A key milestone for FY2008 will be to down-select chemical hydrogen storage materials and accompanying regeneration processes. The chart below illustrates the funding in FY2007 for each major activity along with planned funding in FY2008 based on the Program's budget request.



Majority of Reviewer Comments and Recommendations:

Chemical Hydrogen Storage: Reviewers credited the Chemical Hydrogen Storage CoE with having a good understanding of the key barriers, and a well-formulated, well-focused approach to address critical issues. They stated that the CoE has applied a good mixture of experimental and computational tools and has good collaboration among partners. The CoE has made significant progress in understanding the hydrogen release mechanism in the ammonia borane (AB) system and in increasing both the kinetics and the amount of hydrogen released. However, continued effort is required to further optimize chemical additives and catalysts to increase the storage capacity as well as the kinetics for the 2nd equivalent of hydrogen. Guided by computational analysis, the CoE has developed a potentially energy efficient AB regeneration process. The CoE was also encouraged to continue the search for non-precious metal catalysts, to continue exploring and identifying new promising materials (including non-boron materials), and to maintain their focus on relevant material properties. The CoE was commended for actively applying self-regulating down-selection processes to reject unpromising materials and was encouraged to continue this practice including the narrowing down of regeneration pathways. There are some engineering efforts providing useful guidance for material development. Reviewers also encouraged wider application of up-front system and rough engineering analyses to help identify show stoppers at an early stage and guide material development to address critical issues. The reviewers commended the comprehensive assessment and analysis that was done to identify and rank promising sodium borohydride (SBH) regeneration approaches prior to experimental work. Work related to hydrolysis of SBH for on-board vehicular hydrogen storage will be reviewed in FY07 for a go/no-go decision. With regard to the organic liquid carrier work, it was recommended that systems analysis results be considered while continuing to improve overall capacity, efficiency and kinetics.

Sorbent-based Materials: It was generally recognized that the major accomplishment was the independent verification of metal organic framework (MOF) materials achieving >7 wt.% storage at 77K (MOFs developed by O. Yaghi). The reviewers recommended that DOE fully assess the implications of a cryogenic storage system to evaluate the potential of this class of materials. The other major promising approach is spillover materials, particular R. Yang's work. These materials have shown 1 to 3.5 wt%

material-based hydrogen storage capacity at room temperature and offer a promising avenue away from cryogenic methods. The reviewers recommended that this area of research be expanded to improve the understanding of underlying mechanisms and to improve material synthesis and testing reproducibility. Finally, the majority reemphasized the need to stress materials that lead to near room temperature storage of hydrogen at nominal pressure. Volumetric capacity, hydrogen uptake/discharge kinetics, and durability continue to be hurdles as well. The reviewers recommended that the portfolio be periodically reviewed to ensure that the projects emphasize these issues.

Advanced Metal Hydrides: In general the reviewers found that the Metal Hydride CoE was well-coordinated and organized with good collaborations between center partners. The fact that the center has “organically” down-selected materials which were not found to be promising for reversibility and/or meeting the DOE targets was considered a strength; however it was also felt that a clearer definition of criteria for continuing or discontinuing research on specific materials is needed. Two areas where the reviewers were especially encouraged by the past year’s accomplishments include the use of aerogel scaffolds with destabilized hydrides for lowering desorption temperatures and improving kinetics, and the use of organic adducts to aid in the regeneration of AlH_3 from Al. The reviewers were highly complimentary of the effort to determine the effects of gas impurities on long-term cycling of metal hydride materials and their degradation mechanisms. For the amide/imide materials the reviewers strongly suggested the need for quantification of ammonia release in the desorbed hydrogen. While theoretical modeling calculations were considered highly important and valuable, the reviewers suggested stronger collaborations with more center partners in all four of the key materials research areas and more effort in considering the reaction pathways versus predicted lowest energy end products. Since reaction kinetics is believed to be the major barrier to reversibility for a number of materials investigated, the reviewers recommend greater emphasis on catalyst research. Reviewers were encouraged by cross-center collaboration where expertise developed in one center can benefit the others, such as catalysis and alane regeneration. The majority of reviewers suggested further collaboration, especially with industry.

Tanks: Tank projects were not reviewed in FY2007 due to the reduced effort on tanks. Reviewer comments on the validation of the cryo-compressed hydrogen storage tank project (Lawrence Livermore National Laboratory) are presented in the Technology Validation subprogram of this report.

Testing, Safety, Analysis: These topics were considered critical to the overall subprogram and will be continued as planned. The new project to document best practices in the measurement of hydrogen storage materials was commended by the majority of reviewers. The new area of safety R&D for materials and systems (a new project under the International Partnership for the Hydrogen Economy) was also commended and will be strengthened, with increased coordination among the CoEs and independent projects. The two storage systems analysis projects by TIAX and Argonne National Lab were rated highly. Further refinement of assumptions, continued coordination among stakeholders and developers and validation of models were considered essential.

Note on Storage Report Structure:

Chemical Hydrogen Storage
ST-24 to 30 and STP-8 to 15 are partners of the Chemical Hydrogen CoE.
ST-23 is an independent project.

Sorbent-based Materials
ST-1 to 8 and STP-1 to 7 are partners of the Hydrogen Sorption CoE.
ST-9 is an independent project

Advanced Metal Hydrides
ST-14 to 21 and STP-24 to 31 are partners of the Metal Hydride CoE.

Other New Materials and Concepts
ST-10

Testing, Safety and Analysis
ST-22, ST-31 to 33, STP-36

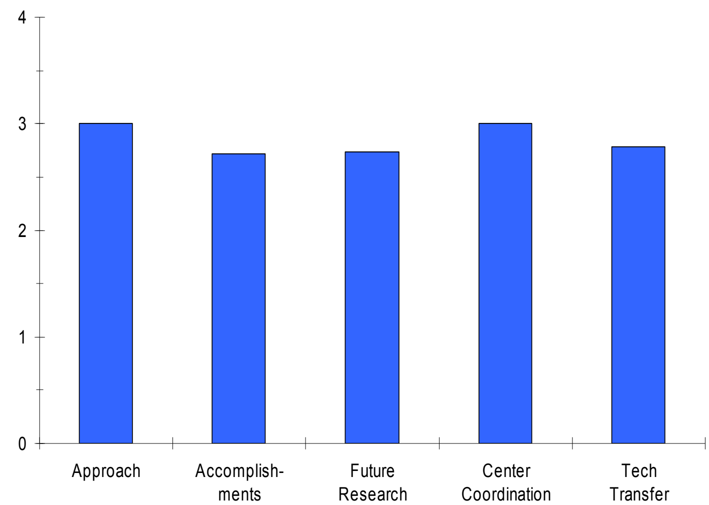
Cross-Cutting
STP-17

Project # ST-01: DOE Hydrogen Sorption Center of Excellence Overview
Mike Heben, Director (presenting); Lin Simpson, Co-Director; National Renewable Energy Laboratory (NREL)

[NOTE: This review was to evaluate the entire Hydrogen Sorption Center of Excellence as a whole. A separate review form was used and can be found in Appendix D**.** NREL's technical contribution to the center is evaluated in ST-02. **]**

Brief Summary of Project

Overall Project Score: 2.8 (7 Reviews Received; 6 provided scoring)



The mission of the DOE Hydrogen Sorption Center of Excellence (HSCoE) is to develop materials that will enable close to room temperature storage of hydrogen on-board a vehicle at moderate pressure. The strategy used by the HSCoE is to design and synthesize materials which bind hydrogen as either (a) weakly and reversibly bound atoms or (b) as strongly bound molecules. Examples include nanoporous polymers, boron/carbon polymers, metal-organic frameworks (MOFs), carbon nanohorns, aerogels, carbon-metal hybrid nanomaterials, new materials "built from the ground up", and new multi-component sorbents. Additional objectives are to understand mechanisms and the interplay between structure, binding, and material stability and storage densities (per volume and per weight) and develop the experimental and computational tools to speed discovery, development and testing of materials that meet DOE system goals.

Question 1: Approach to performing the R&D

This project earned a score of **3.0** in this criterion.

- This CoE has expanded its focus beyond carbon and is actively investigating a set of diverse physisorption materials. These new material classes that are being pursued present promising routes to improved storage properties. There should be more focus on identifying strategies/material classes having higher volumetric uptake (a major barrier typically associated with open, high surface area materials). The go/no-go decision-making process should be more fluid and integrated as a standard part of the program so as to effectively filter out the non-progressive work.
- Sound approach to address technical barriers, moving from theoretical modeling to material synthesis and development.
- Pooling of expertise, facilities; fostering of collaboration and complementary activities. Effective down selection and decision points have been set in the interest of the work. A good mix of technologies and technical capabilities. The CoE has shown the flexibility to change and adjust as new information is obtained.
- Diversified approach with integration where beneficial is a good approach at the high level. Diversification to more low temperature work and addition of other atoms than carbon as substrate is good. Still probably an excess of work on nanotubes and fibers. While go/no-go was mentioned, it does not seem to be an organic part of the program to the extent it is in the entire DOE program or other CoEs – this needs to be in the plan and seen as a good thing, this latter part is not clearly true in this CoE. Clusters are a nice way to organize the work and get more done. Theory guide is appropriate.
- Optimized binding energy and theory-guided research can effectively address most of the technical barriers. The "clusters" research approach is good in general. Too many activities within clusters and only some of them may lead to progress. Need [to] down select certain clusters and redirect the available resources to the most promising materials. Need more balanced and well planned activities among the five "disciplines" to best utilize the available resources.

- Good scope expansion to chemisorption and "enhanced physisorption" on various adsorbents beyond carbons to increase probability of successful development of a system storing hydrogen above cryogenic temperatures.
- Excellent – the PI delivered an excellent talk as usual describing the direction and breadth of work covered.

Question 2: Technical accomplishments and progress toward DOE goals

This project was rated **2.7** in this criterion.

- A significant increase in experimental output was shown which has enabled many more materials to be characterized and tested. Although many of the non-crystalline multi-dimensional materials are often more challenging to characterize, additional focus in this area is encouraged to conclusively determine the identity and understand the mechanism (a key to optimization) for each compound. Theorists should also more closely coordinate with experimentalists to ensure there are rational synthetic routes to prepare promising candidates.
- Good progress and a step forward as demonstrated by the promising data presented on enhanced uptake for specific surface area and by the validation of the spillover concept for developing C-based bridges to increase storage capacity. Materials discovery efforts intensified and led to the identification of a number of promising systems. The complementarities of theory and experiments have widely benefited the program.
- The spillover/bridging work has progressed significantly. The metal-C60's synthesis has progressed albeit the results at this point are a little short. The theoretical/modeling work is moving forward with coming up with new alternatives.
- Excellent synthesis and improving calculation work. Spillover has been confirmed only at much reduced level and remains a big question. Later poster showed confirmation. Synthesis of the fullerenes is excellent chemistry but of unclear value from an application view. Calculations of spillover are very interesting and help support that work more than the experimental work of late. The zeolite template work (outside the center) is very interesting, but needs confirmation. No real progress in the center in terms of capacity since last year on MOFs or spillover, almost the same slides actually. Still cling to the 12 hydrogens in Sc compounds even though results pretty clearly show that mostly cross linking occurs, not hydrogen binding. I believe progress has been better than what was shown in this talk.
- Progress has been made in certain areas. Improved fundamental understanding. All the accomplished materials/systems are still far away from DOE 2010 targets.
- Why is there so much focus on 77K storage? Is it practical? In general, progress of the CoE is good comparing to where it was 2 years ago (issues of reproducing capacity measurements on SWNT). Interesting leads have been demonstrated (e.g., storage by spillover that can be applied to various receptors). Good involvement of theoretical group from Rice. Still, need to speed-up no-go decisions (e.g. on [transition metal] TM-C60 systems).

Question 3: Proposed future research approach and relevance

This project was rated **2.7** in this criterion.

- Good to see expansion of MOF work through addition of new project. It is acknowledged that this CoE faces higher risk, more challenging synthetic routes. However, as much as possible, efforts should be devoted to candidates where there is a rational preparation route in place. Should perform variable temperature uptake for most promising materials to understand capacity-temperature tradeoffs.
- The proposed work is appropriate and it is the next logical step building on current experiences.
- Not clear if more work/resources will be devoted to spillover/bridge systems. Need to use the synthesis and test results to calibrate the modeling/theory (not clear the reverse feedback exists and if so, please give an example).
- Detailed plan. Most topics are appropriate and required.
- Future work plans are indeed built on the past progress. Hybrid material approach should be further explored to cover non-carbon based sorbent. Down select criteria were not well defined. Need to define what the unproductive directions are. Adding precious metal onto carbon is not a good way to overcome the cost barrier. Need to address the cost issue in the future research direction.
- Good proposal for the future involving non-carbon systems as well. Suggest more focus on developing materials capable of storing hydrogen at ambient temperature. Perhaps, conducting a theoretical screening of

potentially new MOF structures with enhanced heat of adsorption (>18 kJ/mol) that would work at ambient temperature.

- Key issues for this center include:
  - Volumetric efficiency – Not enough was highlighted this year (slightly better than last year) every presentation in this center needs to provide brief summary of how their material could reach decent volumetric densities – at least to surpass 350 bar technology).
  - Increasing storage temperature from 77K to room temperature – The center needs to understand that this is a priority and determine a way to report work at conditions of 298K and 350 bar (range more suitable for OEMs).
  - Explaining spillover effect and mechanisms – Many mechanisms were presented that adequately explain the phenomena or provide hypothesis- these hypotheses need to be validated analytically.
  - Explaining deviations from "Chahine rule" – Is it that nitrogen doesn't see all the sites or is there a double layer effect somewhere? This needs to be clarified.
  - Gravimetric storage capacity – Still unacceptably poor at room temperature.
  - Agreement of modeling to synthesis work – Models are providing molecules that are unrealistic to produce or become unstable after a few cycles – the experimentalists need to push back on modelers to provide simpler compounds that have a chance to be made cheaply.

Question 4: Coordination, collaborations and effectiveness of communications within the CoE

This project was rated **3.0** in this criterion.

- All materials synthesis groups/efforts should have access to all measurement/characterization techniques. From the organizational charts, it is implied that only some synthesis groups are actively collaborating with groups possessing specific characterization techniques.
- The project has obviously benefited from pooling of resources. Progress appears to be followed up and controlled for effectiveness. Strong teaming, interaction and joint decision-making is mentioned in the presentation. Nevertheless, clarifications/more transparency may still be needed on how the CoE truly operates, how flexible it is and how its members are involved in the working clusters/groups/disciplines and in the crucial decision process and finally in the execution of these decisions. What is the internal/external information flow mechanism used and which are the terms of reference for the scientific/management board running the CoE (meetings, communication channels, level of participation of partners in the decision making mechanism, etc.)?
- Good communication, coordination and collaboration in general. The University of Michigan seems a bit of a lone program that others chase after to get data, as opposed to an open and willing collaborator.
- Demonstrated some collaboration. Need more collaboration between different clusters. Need to validate the measurement consistency between different groups.
- Good collaboration.

Question 5: Collaborations/Technology Transfer Outside the CoE

This project was rated **2.8** in this criterion.

- External collaborations with other CoEs and institutions appear to be well-developed.
- It is very encouraging to see the first signs of cross-fertilization of results and collaboration within the CoE itself but also across the CoEs.
- Seem to have good connections outside the CoE. Like all CoEs, could do better at communicating with other CoEs to learn both science and management strengths and needs there.
- Need more interactions with research groups outside CoE. Some of the foam materials developed with the center should [be] sent to the Metal Hydride CoE for them to incorporate with their materials.
- Perhaps, opportunity could be to enhance collaboration on MOFs with Yaghi's group [UCLA] as well.

Strengths and weaknesses

Strengths

- Strong, diverse, and competent team taking on high-risk and challenging materials synthesis.
- Partners' areas of expertise very complementary to one another.

- Center's flexibility and willingness to take on new materials synthesis directions.
- Pooling of expertise and capitalizing on lengthy experiences in diverse fields.
- Good mix of theory/modeling and experimental work.
- Good pipelines of theoretically developed alternatives.
- The center management has shown flexibility and ability to change and adjust.
- Good team, good synthesis skills, Rice adds some good theory.
- Focused on fundamental understanding and bottom-up design.
- Area of adsorbents (enhanced physisorption and weak chemisorption) can potentially result in a winning storage material with enhanced storage energy efficiency (e.g., versus metal hydrides).

Weaknesses

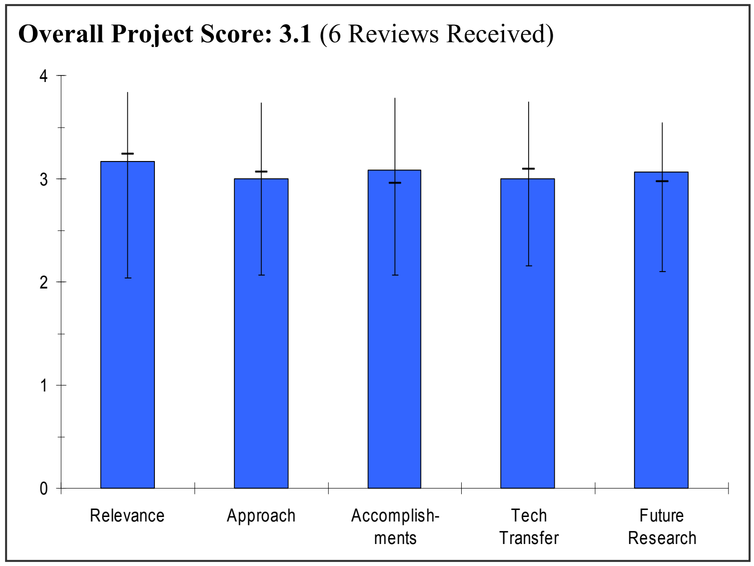
- Experimental realization of targeted materials limited by their complex nature and non-intuitive syntheses.
- Go/no-go decisions seem to be externally applied and not part of the internal CoE process. Regular go/no-go decisions are important for ensuring that projects are progressing.
- The challenge of managing such a broad R&D portfolio involving so many and diverse research groups.
- Need to develop benchmarks for C60s and their derivatives.
- Feedback to the modelers to adjust after receiving actual data.
- Still too committed to original themes. Complex calculations continue to be done in absence of interactions with other fullerenes.
- Validation of some critical experimental results that might set future directions.
- There is no clear plan on how to move some of the promising work forward.
- There is no plan on how and when to make go/no-go decisions.
- Significant focus on storage materials at cryogenic temperatures.

Specific recommendations and additions or deletions to the CoE scope

- Future work could strive for a better balance between modeling and synthesis/testing.
- Operability/workable conditions need to be always kept in mind – adsorption must be addressed to occur close to ambient conditions rather than cryogenic temperatures (77K).
- Volumetric capacity is a critical issue and needs to be appropriately addressed.
- Enhance the interaction with related projects and international partners (outside the CoE).
- Agreement should be reached on reporting of adsorption data (e.g. total/excess/absolute uptake).
- More emphasis on validation testing.
- The most recent results from spillover/bridged materials warrant further resources to be devoted to this approach. NREL could provide much help to work on ways to improve the kinetics of the room temperature (RT) sorption.
- It is very important that the theory team, that have been doing the decorated C60, back up and learn from previous predictions vs. reality. Take, for example, the prediction that many TM atoms can be placed on C60, reality allows only one, they need to figure out why and adjust methods. Likewise they continue to do the calculation for a lone C60, but as was predicted by reviewers, the C60s crosslink through the metal atoms. The theory team needs to start making the calculation to see not only if the metal is stable on the C60, but also if there is cross-linking and can hydrogen still attach, otherwise the calculations are of much less value.
- Reorganize some of the research activities and focus the available resources to the most promising materials.
- Analyze data from all the "clusters of accomplishments" on the same basis, that is put all capacity plots in the form of isobars (e.g., at 100 bar), and see which materials are more selective towards storage at ambient temperature. This may help in selecting most practical materials that may not show all benefits at 77K.
- The center has adequate level of internal milestones and go/no-go decisions - however it seems only by force that they are implemented. The biggest disappointment of this center is that they are slowly moving back towards carbon nanotube and fullerene compounds. These compounds are expensive to make and their methods seem to employ complicated methods to functionalize these compounds. How could this ever be cost effective and scalable? Progress on MOFs and novel concepts were nonexistent this year. This center perhaps more than any other center has more opportunities for novel technologies that they are not fully looking into. They really need to take a deeper dive into the capabilities of organometallic chemistry and look to other industries for inspiration such as the medical and semiconductor industries.

Project # ST-02: NREL Research as part of Hydrogen Sorption CoE
Anne Dillon, presenting; J. Blackburn, C. Curtis, M. Davis, C. Engtrakul, M. Heben, K. Jones, Y. Kim, K. O'Neill, P. Parilla, L. Simpson, E. Whitney, S. Zhang, Y. Zhao, NREL

[NOTE: This review is for NREL's technical contribution to the HSCoE.]



Brief Summary of Project

NREL is performing R&D and coordinating the Hydrogen Sorption Center of Excellence (HSCoE) to develop the applied science base and technology advances required to meet DOE's on-vehicle hydrogen storage targets. In FY 2007, NREL's research efforts have been refocused to:
• Using theory as a guide, actively pursue the synthesis of new promising compounds for reversible hydrogen storage with desired binding energies.
• Determine structures of new compounds and correlate the structure with adsorption mechanisms, desired binding energies and capacities (volumetric and gravimetric).
• Employ theory to explain and confirm observed experimental results as well as to establish optimized structures that have rational synthesis routes.
• Expand hydrogen capacity measurement capabilities for rapid screening to improve round robin process / sample exchange with partners.
• Continue theoretical efforts to predict / design new sorption materials consisting of light elements but not restricted to a carbon base.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.2** for its relevance to DOE objectives.

- Carbon-based adsorbents represent a viable option toward reaching the DOE objectives and thus, this research is aligned appropriately. The experimental targets (based on theory) for this project, however, are challenging and ambitious ones. Due to the complexity of these compounds, a great deal of time/effort will likely be devoted to trying to isolate, purify, and scale-up these materials.
- With ideal packing, the volumetric density of the majority of these candidate materials (for example, organometallic fullerenes) will not be close to achieving the 2015 volumetric target. This should be a primary focus for future materials selection.
- The sorption research is a critical approach to developing storage materials.
- The technical effort was redirected after the single-walled nanotubes (SWNT) go/no-go decision. New research directions generally support the DOE goals, but all approaches are high risk.
- The project directly addresses the DOE storage objectives. The presentation did not address directly how storage system targets will be met. It did not address either how Barriers A, C, E would be or have been addressed.
- Relevant to a greater extent now that they see their calling as physical adsorption rather than nanotube - fullerene adsorption.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- In principle, the approach is good, using theory to help guide the identification of experimental candidates. However, for many of these targeted compounds, it is still not entirely clear that there are rational synthetic pathways to their preparation. It is good that there is a heightened focus on experimentation that is helping to drive this project's potential success. In terms of theory, full evaluation of the stability of current and future structures should be routinely performed.
- A good mix of theory, synthesis, testing. Also showed flexibility to change and re-adjust approach.
- Multiple theoretical approaches for enhanced hydrogen adsorption are being pursued. There is a robust link between theory and simulation and materials synthesis and testing. This interaction allows timely evaluation of new concepts and predictions. Strong chemical synthesis capability is enabling the development of new carbon-based materials with potentially higher surface area and binding energy. The emphasis on OM-fullerene compounds (reactivity and sorption enhanced by metal on the fullerene) and B-doped SWNTs with higher binding energy for hydrogen—good extension and re-direction of work from 2006. Excellent characterization and analysis tools and capabilities support the synthesis effort.
- Clear focus of the research. Although the interesting results are mainly theoretical, the researchers are striving to the experimental realization of the compounds. Issues and problems were addressed frankly. Project plans retroaction between theory/experiment. The technical targets A, C and E were not addressed in the presentation.
- Theory guide is a good idea but it needs to be noted that the theory was isolated clusters, and others have correctly suggested 'chains' would occur several years ago. The theory does not seem reliable enough to really be a guide - They need to go back and figure out why the metal was predicted to put many atoms on a buckyball and only one goes on, and change the approach to get the right answer. Also need to calculate in an environment where balls can cross link. Movement toward non-carbon systems is wise.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.1** based on accomplishments.

- While an increased focus on synthesis has clearly been demonstrated, unfortunately not too much progress toward making the specific candidate materials has been shown, although the experimentalists are not faulted for this as the synthesis targets are extremely challenging. In general, there should be more focus on identifying experimental candidates for which there are known synthetic pathways.
- Good progress on synthesis albeit the actual results came short. Good continued work on the theory to guide future work.
- No significant progress.
- Impressive progress on OM-fullerene synthesis (NREL has successfully addressed a very difficult synthetic chemistry challenge). New results on Fe-containing fullerene are intriguing. However, there are serious concerns: binding energy is still too low; reactions involving multiple hydrogen adsorption/desorption cycles may likely be influenced strongly by contaminant poisoning and by fullerene-fullerene interactions and metal agglomeration. Also, it is surprising that the binding energy with hydrogen seems to be similar for different metal species. Enhanced hydrogen adsorption in B-containing SWNTs certainly is an encouraging result. It will be important to understand how hydrogen uptake scales with B concentration. Does simulation/modeling allow an estimate of maximum uptake that might be expected from B-doped materials (including the new metalloboranes)? New theory work on endohedral metallofullerenes suggests higher binding energies and enhanced uptake seems promising. Temperature dependence of sorption properties needs to be quantified.
- Excellent theoretical results - more experiments needed! Enhanced binding observed in metal doped materials. Experiments tend to lower expectations from theory. It is not clear how barriers C and E can be addressed within this project.
- Excellent synthesis work. The compounds are coming out fast - though the storage is low the temperatures are interestingly high. Li system did not clearly have much capacity at present but again a nice synthesis achievement form a science perspective. B work is a good idea though no progress yet in capacity; still this is a good thing to pursue some more to see what possibilities it has. At 1000K the metallocarboranes do not sinter the metal, but will multiple fullerenes agglomerate at realistic operating temperatures? Rapid screening equipment is a nice technological accomplishment. Consider also that they have over 2 million dollars to achieve this; otherwise they would get a higher score.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- NREL is clearly supporting the sorption CoE greatly in providing measurements/consultation to various institutes. The personnel behind this project are an ideal combination of experimentalists and theorists leading to productive internal collaborations. Additional communication with the Rice group is encouraged regarding the C60 linking work as to avoid potential overlap.
- Theory is important to guide the experiment. But the opposite must happen too. In some cases the theoretical predictions look very hypothetical. A closer collaboration between theoreticians and experimentalists should take place.
- Good collaboration with other experimentalists and theorists both within the HSCoE and with the external technical community. This is definitely an activity that can benefit from collaborations across the entire HSCoE.
- Cross-collaboration looks excellent although it did not come through clearly (i.e. role of various partners) from the presentation. Very nice theory/synthesis/sorption property measurement integration.
- Well connected and using connections effectively.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.1** for proposed future work.

- Proposed future research directed at investigation of simpler systems and chemical transformations is important toward experimental realization of intended more complex structures. However, hopefully these studies will not lead to an in-depth basic science research project which will detract from hydrogen storage materials research.
- Increased focus on conclusive structural determination is recommended.
- Development of rapid throughput of hydrogen storage capacity measurements is valuable for efficient materials testing and supports the sorption CoE partners.
- What is the approach for room temperature sorption? Cr-C60s? What are the benchmarks for C60s or metal-C60s? What results warrant more resources or vice-versa?
- 1 & 4 look very promising 2 & 3 not; but they needed for the final decision of the existence of these systems.
- Future work is a good extension of the efforts initiated in 2005/2006. Addition of new reactor(s) that enable higher B concentrations will be useful. Recommend additional modeling work that provides projections of hydrogen sorption properties at higher temperatures; and simulates how interactions among metal-containing carbon frameworks during hydrogen cycling will influence sorption behavior.
- Clear research objectives. Go/no-go decision on SWNT. The project's objectives have been refocused.
- Plans seem OK but I wonder if there really is a plan to get out of the C60 work if they can not see a route over 1%.

Strengths and weaknesses

Strengths

- Implementation of both theory and experiment is an ideal approach toward hitting a “homerun”. Expertise in these areas is clearly evident in this project, and there now seems to be a good balance in research effort allocated toward both.
- Strong theoretical basis.
- Also combined with a lot of synthesis work.
- Very strong theory/modeling and synthetic chemistry effort. The NREL team is attacking difficult technical problems in an innovative way.
- Excellent work being done to experimentally test predictions derived from theoretical work.
- Excellent synthesis work shows the team's ability to seek new materials for sorption storage.
- The team is strongly motivated to validate theory experimentally.
- Team clearly exhibits its capacity to refocus and push promising alternatives.
- Exciting theoretical results.
- Outstanding work overall.

- Right energy range, good synthesis abilities. May generate higher temperature cryosorbents with the higher energy materials if the specific surface area (SSA) can be increased to where it "should" be.

Weaknesses
- A clear path to experimental realization of the theory-driven structures is not apparent.
- There needs to be more focus on strategies which enable these materials to reach the 2015 volumetric target.
- Not clear the pathway for RT sorption.
- C60-M-[C?]5H5 LDA theoretical calculation is not the state of the art, and due to symmetry not appropriate.
- The existence of metallaborane nanostructures is not proven yet. At some point the theoretical design must be also be guided by experimentalists.
- All approaches being pursued here are very high risk and involve fairly exotic materials and processes. This is not necessarily a weakness *per se*, but it is important that the ideas aren't "oversold" — i.e., a careful assessment of the large gap that currently exists between the proposed and demonstrated materials properties and the DOE goals must be made (i.e., what are the big roadblocks in getting from "here" to "there"? Is an incremental progress path acceptable or is there a discontinuity that requires an entirely different research approach?) The NREL effort would be enhanced greatly if this analysis and possible proposed mitigation strategies were made available to the community.
- Experiments still lag theory although noticeable efforts have been made.
- Cost issues not addressed.
- Still seem to be looking for a way to make SWNTs be the answer with no real success or justification. This probably holds the program back.
- Theory is holding the program back by predicting unrealistic things AND failing to go back and change the approach. The buckyballs MUST be calculated with the option to cross link. The theory needs to go back and figure out why they predict lots of metal atoms and reality allows only one.

Specific recommendations and additions or deletions to the work scope

- Clear decision-making points for continuing/discontinuing work on decorated C60 should be set. At what point is it time to move on?
- Need to develop benchmarks for various alternatives specifically the x-C60 and in general any molecules under consideration.
- Perform C60-M-C60 calculation in the LDA level and C_5H_5-M-C_5H_5 in MP2 and compare the results. Only in this way they can have size and method accuracy.
- Recommend de-emphasizing work involving highly reactive "bare" metal atoms on a C-framework structure. Although these structures may have encouraging performance from a theoretical standpoint, it is not likely that they will remain intact in their original reactive condition after multiple cycle processing.
- Less nanotube work; more non carbon work, more low temperature work.

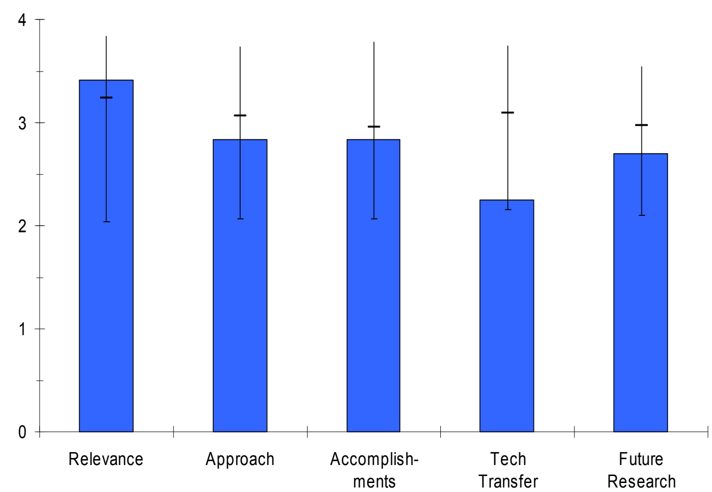
Project # ST-03: Hydrogen Storage by Spillover
Ralph Yang; University of Michigan

[Member of the Hydrogen Sorption Center of Excellence]

Brief Summary of Project

The overall objective of this project is to develop carbon-based hydrogen storage materials with capacities in excess of 6wt.% and 45 g/L at room temperature. This will be done by developing and optimizing new bridge-building techniques for spillover to enhance hydrogen storage. This will result in a mechanistic understanding for hydrogen spillover in nanostructured carbon-based materials for the purpose of hydrogen storage.

Overall Project Score: 2.9 (6 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.4** for its relevance to DOE objectives.

- Concept of spillover could potentially be important towards taking sorbents from 77K to room temperature operation.
- Seems to be making negative progress (last year's results are "not reproducible", lower weight percents reported this year, no volumetric densities reported?)
- Don't know what this means that "desorption is enough to power a vehicle at 60 mph". DOE has set targets for hydrogen desorption rates – why hasn't the PI simply compared with these kinetic targets?
- Very promising mechanism.
- Room temperature hydrogen storage in a sorbent material is very relevant.
- The PI uses a novel bridge-building technique where catalyst supported on a receptor surface dissociates the hydrogen molecule and enhances sorption through increased diffusion. Understanding of the cluster / particle — support interaction is critical.
- This project has high potential to meet gravimetric and volumetric targets and possibly charge and discharge rates as well.
- If this can be shown to be real in the case of MOFs, then this is well aligned and important. If only the 1.2% on AX21 is real, then this work is not in line. As last year, external confirmation of high storage amounts is key.

Question 2: Approach to performing the research and development

This project was rated **2.8** on its approach.

- Like almost all the work in the sorbent area, this work needs to strongly focus on: 1) increasing binding energy to enable room temperature storage, 2) increasing gravimetric capacity, and 3) increasing volumetric capacity. All three must be achieved simultaneously.
- No sufficient theoretical explanation of the spillover phenomenon.
- Kinetic issues are being addressed.
- The PI is developing and optimizing the bridge-building technique by directing doping of the receptor.
- It is not clear what the approach will be to increase the hydrogen adsorption rate. Since this is a very promising approach, perhaps the HSCoE could be used to provide input for a broader perspective on future direction.
- Spillover is valid and real mechanism in chemical processing. Verification that this is really happening by some mechanism - say verifying H atoms on the surface, is still a very important task to prove that they are spilling

onto the substrate. Addition of the parallel calculations work is a big plus for this program. Needs to use a MOF that won't degrade; this is pretty clear, MOF-177 is not a good choice. Not apparently thinking about lowering Pt loading (way too expensive), need a better plan.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.8** based on accomplishments.

- Seems to be making negative progress (last year's results are "not reproducible", lower weight percents reported this year, no volumetric densities reported?)
- In general, the mechanism that is used to describe spillover seems to be a “kinetic” argument; however, the PI states that the effect is actually thermodynamic. Is there a contradiction here?
- Modeling results do not seem to agree with 20-25 kJ binding reported experimentally; however, PI claims that the results agree? Taking an average of the theoretical results for binding energies is simply not appropriate: a system with half of the sites with ~0 binding and half with ~40 kJ binding will behave completely differently from a system where all of the sites have ~20 kJ binding.
- At last year's meeting, there was a significant issue raised concerning the incompatibility between the proposed explanation of spillover and the proposed thermodynamics of spillover. The PI did not address this very serious concern in his presentation.
- Explanation for the lack of reproducibility of the MOF results was not convincing. It is likely that the method used to process the MOFs in this group (which is different from what other groups are doing) could be the source of the variability in the results.
- Not much progress from last year.
- How likely is it that the 2007 target of 4.5 wt.% will be met at room temperature with AX-21? Have all avenues for addressing the issues of MOF instability and reproducibility been pursued? Are MOFs being deemphasized prematurely?
- A number of receptors such as IRMOF-8, and activated carbon have been tried with significant improvement in hydrogen storage capacity. The experiments are well-coordinated with theory.
- These materials show great promise for meeting the DOE targets. It is clear the principal investigator is conducting his research with the DOE targets in mind.
- Technically this moved backward. However that dose of reality was needed in this project. The PI needs to be more open and share this program. There is rising doubt as to the reality of the 4% result. The binding energy was a very good thing to accomplish. Many of the slides are direct holdovers from last year.
- The calculation of hydrogen potential based on adsorption on all atoms was very speculative.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.3** for technology transfer and collaboration.

- PI could really benefit from close coordination with groups with more substantial expertise in MOF synthesis.
- Seems like this project is a little short on technology transfer and collaboration. Perhaps collaboration could help with the issues associated with IRMOF-8. Collaboration with spillover modeling being done at Air Products would be desirable.
- The project is well-coordinated with other groups/institutions/laboratories working on the project.
- Since this is such a promising approach, it would be good to see more interaction and parallel or complementary work at other institutions.
- This program has been secretive up until this year. Addition of parallel Rice work is very good, but the two programs seem virtually unconnected other than by Rice attempting to justify the published data. This still appears that it is not a collaborative or open program. It would be much more effective in moving forward if it incorporated other people and teams.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.7** for proposed future work.

- It is not clear how the PI will get beyond the ~1 wt.% he reported this year at room temperature. What is the strategy to improve the storage capacity?
- PI wants to achieve 4.5 wt.% "system" level target in FY2007. This would require a nearly one order-of-magnitude improvement over the 1 wt.% results presented here. What is the strategy to achieve this (within the next few months)?
- Very good idea of performing spillover in MOFs and MILs and COFs.
- It is very important to obtain basic understanding of the spillover process including equilibrium and kinetics, using deuterium isotope.
- If AX-21 and other high surface area carbons do not have sufficient hydrogen capacity, is there a "Plan B"?
- The PI plans to study different receptors (MOFs, COF-1) and catalysts as well as direct doping techniques to achieve DOE targets. Also the future plan is a basic understanding of the spillover process.
- I would like to see a tabular description of what the future plans are for new MOFs, doping, and receptors.
- The proposed work is not inappropriate, but largely ignores the real questions of why no one can reproduce the 4% result, seemingly not even them, and why no one has shown conclusive evidence that H atoms are on the surface. Ignoring these critical questions is not appropriate for a managed program. Of the planned work the deuterium scrambling experiment may be the best. There is little detail to the plans and the program seems to move by response to observations not by intention or plan.

Strengths and weaknesses

Strengths
- Hydrogen storage at room temperature.
- New spillover mechanism for hydrogen storage.
- The spillover mechanism is a novel approach, and optimization of both catalysts and receptors may yield the derived storage material.
- Good science.
- Excellent focus on DOE targets.
- Promising results.
- Concept has great promise if it is really working and it is based on a known technology. The energy appears to be in the right range and the system works at room temperature.

Weaknesses
- The spillover mechanism is not understood yet.
- It would be nice to have more insight into why the spillover mechanism provides for room temperature hydrogen storage, whereas other sorbents only show significant hydrogen storage at 77K.
- The PI's reluctance to talk about the doping technique or dopants makes it difficult to assess its effectiveness. No discussion was provided on the line of thinking that makes one select the dopants, catalysts, or receptors. Poor understanding of why certain results are irreproducible. The basic understanding was poor.
- Since this work is so promising, I would like to see parallel and/or complementary work conducted at other sites.
- Program has done little to prove it is accomplishing what it claims (making atomic hydrogen on surfaces), and progress has been slow or backward since the initial claims. Not very forthcoming with those hoping to verify results or help them with their work, as best as we can see.
- This is one that has high potential and low performance for a year or more, the center or the DOE needs to step in and tune up the plans and improve the output of results.

Specific recommendations and additions or deletions to the work scope

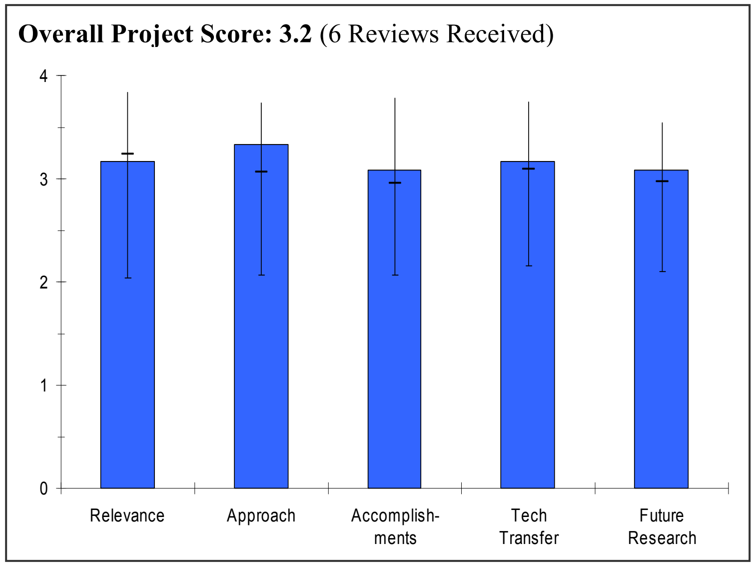
- None.
- Emphasis should be placed on fundamental understanding of the spillover mechanism.
- This program desperately needs to reproduce the MOF result on an air stable, ultra high surface area substrate. I would avoid unstable MOFs no matter how high the surface area. There are air and water stable MOFs available and refusal to try stable substrates is tantamount to admitting the 4% result is erroneous.

- The program needs to verify spillover is occurring by direct measurement. If need be by forming the hydrogen layer in a chamber attached to UHV tools by a gate valve, then quenching to low temperature to maintain the hydrogen layer and moving into a vacuum chamber to observe the state of hydrogen in EELS or other tools sensitive to atomic hydrogen bound to surfaces.
- To be clear, this area of work must be continued because it has much promise; but there is a need to direct it in a much better way. To prove H atoms are made, verify that the theory is correct by testing it in a system the theory was not fit to, and verify that the failure to reproduce is due to the MOF stability, not poor measurement.

Project # ST-04: Theoretical Models of H_2-SWNT Systems for Hydrogen Storage and Optimization of SWNT Production

Boris Yakobson, presenting; Robert Hauge, co-PI, Rice University

[Member of the Hydrogen Sorption Center of Excellence]



Brief Summary of Project

Rice University is developing predictive models of material's interaction with hydrogen, in order to optimize their makeup for storage and assess the gravimetric and volumetric capacity. Rice will provide recommendations for the synthetic goals (e.g. diameter, type and organization of nanostructured materials). In 2007, Rice is preparing synthesis of metal- and electronegative group (F, BF_3) enhanced VANTA (vertically aligned nanotube arrays, contrast to fibers) for H_2 adsorption. They are also working on the theory of hydrogen spillover, its thermodynamics and kinetics: energy states, cooperative effects, and mobility.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.2** for its relevance to DOE objectives.

- Cryogenic sorbent materials are not likely to achieve the overall DOE objectives. Spillover or metal-doping to increase binding energies are two possible candidates for moving these sorbent materials to room-temperature storage. However, neither has really been reproducibly demonstrated to any significant capacity. Thus, it is not clear that the focus of this project is really in support of the overall objectives of the HFI.
- The methodology is interesting but the materials are not very promising for hydrogen storage.
- The objectives of this project support the DOE Hydrogen Fuel Initiative and R&D objectives in general. Connection to Yang's work at UM is valuable and has potential to yield suggestions for optimized systems.
- The PI is carrying out state-of-the-art calculations to understand the spillover mechanisms on a variety of systems. This understanding is essential for optimizing the catalysts and the support.
- This project would be more critical to the Hydrogen Initiative if carbon based materials, in general, had a reasonable chance of meeting even the 2010 storage "system" goals which will very likely require a materials storage capacity of at least 10 wt.% H to compensate for the balance of system components. The project generally supports the DOE RD&D vision for hydrogen utilization in vehicles by providing important insights into performance controlling issues for hydrogen storage materials, like binding energy parameters, additive aggregation, and spillover.

Question 2: Approach to performing the research and development

This project was rated **3.3** on its approach.

- The approach is interesting. Nevertheless studying spillover on surfaces is not a good approach.
- Approach sounds good in concept and is focused on technical barriers. The approach on spillover [effect] can be improved to predict the optimum receptor properties. Suggest to further explore accuracy of quantum chemical (and density functional theory [DFT]) predictions by validating with experiment.
- The PI is well aware of the limitations of the DFT and is using appropriate techniques to deal with dispersive forces. The barriers for diffusion are being calculated correctly.

- The engineered 3-D foams, vertically aligned nanotube arrays, and cross-welding studies are fully consistent with the direction that research on carbon-based storage materials needs to take. The theoretical studies of the adsorption energy landscape constitute an inspirational piece of work that should widely benefit those working in the Hydrogen, Fuel Cell and Infrastructure Technologies (HFCIT) storage program.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.1** based on accomplishments.

- "Welding" of tubes and theoretically-predicted "foams" is an interesting idea, but wasn't this already presented at the last meeting [FY2006 APR]? Very interesting idea/mechanism proposed to explain the "thermodynamic problem" raised at last year's meeting. However, it does raise the question of how do these regions of high-level loading nucleate in the first place? What is the nucleation barrier, and is it plausible that one could overcome it with temperature? Could it be a heterogeneous nucleation mechanism (i.e., on defects in the structure)?
- No significant progress from last year!
- Demonstrated a best foam structure for better hydrogen storage. The recommendations from modeling should cover several scenarios rather than only the best case scenario.
- Effectiveness of computational calculation for [carbon nanotube] CNT-H_2 systems is shown well. Interaction between CNT and H_2 has been clarified with their technique. However, a solution to avoid aggregation of metal atoms is not proposed.
- The PI has demonstrated that metal atoms on carbon support aggregate, adversely affecting hydrogen storage. This effect has already been demonstrated by others, but the PI does not seem to be aware of it. An understanding of spillover kinetics is provided.
- The computational aspects of this program define pathways to improved performance and to overcoming technical barriers to meeting program targets. The carbon materials synthesis work focuses on aspects of carbon nanostructure development that seem appropriate if carbon in some form has any chance of meeting H-storage system targets, i.e., increasing dimensionality, reducing "dead" space, and optimizing spillover.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.2** for technology transfer and collaboration.

- Need to collaborate more with experimental group so that the results from this project can be used by others. Most of the time, theory-predicted optimized condition can not be achieved experimentally. The modeler needs to consider the feedback from experimental group and put them into the modeling assumption.
- The PI works effectively with experimentalists and the work is well coordinated with other members of the group.
- It seems that workers in the HFCIT H-storage program are picking up on the implications and general usefulness of the results in FY 2007. Those that haven't soon will to be sure. Collaborations with NREL, Air Products and NIST are ongoing. Others with the University of Michigan and the University of Nevada Las Vegas are emerging with good reason. One should expect even more to follow.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.1** for proposed future work.

- Like many of the results in this field (of sorbent materials), theoretical predictions far exceed what has been currently synthesized. For the 3D-foam results, the likelihood of synthesis should be critically assessed before investing a lot of time and effort in doing more detailed MC simulations. The work on spillover has proved fruitful, and should help provide a mechanistic understanding which can be either proved or disproved experimentally. Not clear how the metal-doping work will significantly add over the analogous work that is currently going on at NREL.
- The spillover model is not correctly formed. Spillover cannot be studied in a single layer graphitic surface.

- Plans are built on past progress. Need fundamental understanding and experimental validation of the spillover dynamic effect. Suggest omitting the pure carbon VANTA/foam MC simulations as binding appears to be too weak unless metal hetero-atoms are incorporated.
- The proposed future work for the most part represents a logical and appropriate extension of what was reported at this Peer Review. The entire hydrogen storage program would benefit from an expansion of the adsorption landscape energetics computations to include other types of storage media where spillover could come into play. If the optimum spillover architecture is now known, it is then necessary to prove that it can be constructed and maintained (e.g., against agglomeration). Systems with H/C > 1.0 need to be emphasized.

Strengths and weaknesses

Strengths
- Theory prediction can effectively direct the experimental design to achieve the optimized material properties.
- Their extensive experience in computational technique.
- Interaction with people on experimental side through the CoE activity.
- Good understanding of experimental needs and sound theoretical approach.
- The presenter is very knowledgeable and perceptive about how to attack the issues without doing lots of meaningless physicochemical measurements.
- The project integrates considerations of both thermodynamics and kinetics. That's important because both are in play in the hydrogen storage “game”.

Weaknesses
- C_nH_n is a hydrocarbon model and not a model for H @ C material.
- Lack of communication with experimental group to address the technical feasibility.
- The PI should do a better job in handling van der Waal's interaction and be more critical of commercial packages.
- At the present level of funding, progress may not be as rapid as it deserves to be in the coming years.
- Otherwise, there are no obvious weaknesses.

Specific recommendations and additions or deletions to the work scope

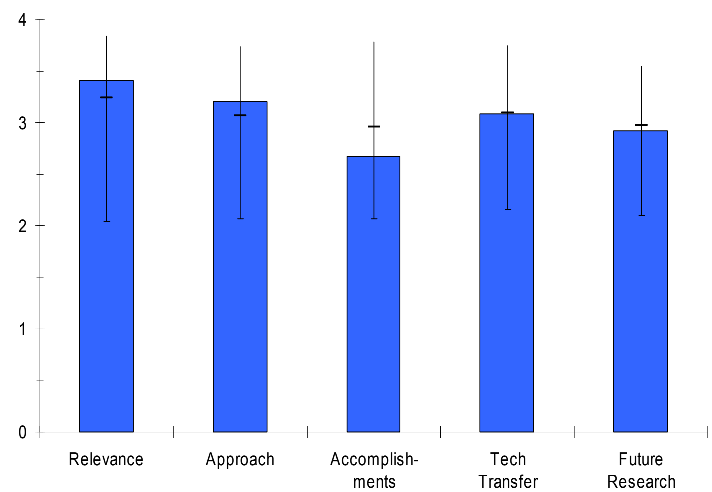
- Suggest adding some study on the effect of different nano pores and channel orientation rather than 1-D structure.
- The entire H-storage program would benefit from an expansion of the adsorption landscape energetics computations to include other types of storage media where spillover could come into play.
- If the optimum spillover architecture is now known, it is then necessary to prove that it can be constructed and maintained (e.g., against agglomeration).
- Systems with H/C > 1.0 need to be emphasized.

Project # ST-05: Cloning Single Wall Carbon Nanotubes for Hydrogen Storage
Jim Tour, presenting; Carter Kittrell, Co-PI; Rice University

[Member of the Hydrogen Sorption Center of Excellence]

Brief Summary of Project

Overall Project Score: 3.0 (6 Reviews Received)



The overall objective of this project is to develop nanostructures and nano-engineering processes that enable synthesis of hydrogen storage materials that can be used to meet the 2010 DOE gravimetric (6 wt.%) and volumetric (45 g/L) system goals, with excellent uniaxial thermal transport properties. This will be accomplished by developing processing techniques to produce specific types of nanomaterial structures with increased available surface area. In 2007, the objectives of this project are:

- Investigate the 2-times steeper slope for "Chahine rule" for H_2 uptake and the concept of high temperature condensate. Determine uptake properties of the precision sp^2 pore.
- Develop alternative spinning methods and solvent extraction methods to increase available pore volume.
- Develop non-acidic lithium/ammonia based fiber expansion and cross-linking methods to circumvent oleum acid extraction problems and generalize the nanoengineered sp^2 pore methodology.
- Begin development of lithium intercalation of rigid nanotube scaffold for Kubas-type binding of H_2 at ambient temperatures.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.4** for its relevance to DOE objectives.

- This project represents one of the more promising experimental work/approaches toward achieving the DOE objectives for this class of carbon-based physisorptive materials. The design strategy (of linking SWNT [single walled carbon nanotubes] into a 2- or 3-D scaffold) and ability to modify these structures (through linker functionality/geometry or dopant additions) distinguish this project and reveal a new avenue toward potentially achieving the goals of the DOE RD&D plan using SWNT as structural building blocks. It does, however, seem as though this project is still in more of a research stage.
- Nanoengineering seems to be the only solution to hydrogen storage problem. Cloning nanotubes (NT) is a very interesting idea. Cloned NTs decorated with metals look [like] promising materials for hydrogen storage [because of] pi-systems, large surface areas and metal binding sites.
- The project scope supports DOE H_2 initiative and overall R&D objectives. The rigid scaffold developed from cross-linking methodology may generate some promising results and lead to a new direction.
- Cost targets seem to be difficult to achieve using SWNT.
- This project is well aligned with the "hydrogen vision" for carbon based materials. It's focused on the intelligent design and synthesis of carbon-based structures containing many of the characteristics that are generally regarded as being beneficial for hydrogen storage by a sorption-type material, namely, a compact, three dimensionally interconnected, high effective surface area, small pore size architecture with under coordinated metal atom inclusions or a similar hydrogen attractor.

Question 2: Approach to performing the research and development

This project was rated **3.2** on its approach.

- Designing chemically 'cross-linked' SWNT is novel approach toward creating multi-dimensional materials having uniform pores whose size, shape, and chemical composition can be modified through linker geometry/length, chemical functionality of pores, and/or addition of dopants. Such control over the size/chemical make-up of the pore structure is important for property optimization. More clarification on the characterization is advised. For example, how uniform/predictable is the degree and location of cross-linking? Has the pore size distribution been performed to ensure that uniform pores have been created? What characterization methods are being used to determine the structure type (i.e. distinguish different potential 2- and 3-D rod-packed structures)?
- Cloning nanotubes is a very interesting idea. Cloned NTs decorated with metals look promising materials for hydrogen storage since pi-systems, large surface areas and metal binding sites.
- General approach is novel. Using model system to study the pore size effect is a good strategy. The cost barrier was not addressed in the approach.
- Approach for solvent removal is a critical item and the activation procedure and absence of residual solvents need to be illustrated prior to hydrogen uptake measurement. Cost targets could be hard to reach.
- The approach embraces just about all the accepted notions regarding what has to be done to achieve DOE RD&D storage targets with a carbon-based material. The research seems to be well thought out and skillfully performed.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.7** based on accomplishments.

- While the approach seems solid, the current progress and results for the synthesized materials are unclear. For example, only slide 9 pertains to hydrogen capacity, and it is not clear which specific samples those graph points correspond to. Need clarification on which samples have been synthesized, which have been tested, and how they perform. Additionally, other examined properties, in particular, the volumetric capacity and kinetics should also be included. In general, more emphasis should be placed on property evaluation for the synthesized materials and an understanding of why certain materials performed better/worse than others (develop structure-property relationships).
- No significant progress from last year. Li does not perform Kubas binding.
- Demonstrated some progress and achieved some promising results. Need fundamental understanding of the material behavior.
- They have not achieved the 2010 target based on their approach. However, it is important for development of materials for hydrogen adsorption that they prove enhancement of heat of carbon material-hydrogen interaction.
- Since the initial results show 2-times slope vs. “Chahine rule,” focus is recommended on increasing the surface area which would be by opening the tubes and optimization of the cross linker for porosity control. Hydrogen uptake results need to shown at room temperature.
- Results were presented that exceed the “Chahine” predicted surface area rule—a step in the right direction. They tested and/or developed some new synthesis methods for cross-linking and lithium addition. They created a new 3-D nanoengineered carbon scaffold. They may be leaning a bit too hard on their extrapolations. Better to get results that leave no doubt about their ability to achieve 6.5 wt.% H and 55 g/L.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.1** for technology transfer and collaboration.

- Work within Rice seems to be diverse and strong. Collaboration with NREL also appears to be a valuable component of their research in terms of testing, and hopefully this relationship will produce even more property data. Additional communication with NREL is important in regards to the C60 linking work, as to avoid duplication of research.
- Certain coordination within the center exists. Need communication with other CoEs to see whether this foam structure can be used by other centers, such as the metal hydride CoE.
- Suggest more collaboration with theoreticians within the center to better select appropriate cross linkers to control the porosity.
- Other than their colleagues at Rice University (Yakobson et al.), it isn't clear how much meaningful interaction they have with their other stated collaborators in the Sorption CoE. Perhaps they should spell this out more clearly in future years.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.9** for proposed future work.

- As indicated in their future plans, more testing of properties (H_2 uptake, binding energy, kinetics, cycling, etc.) on the various synthesized samples, structure-property relationship determination, and continued work on scale-up would be highly valuable.
- The nanotube scaffold idea looks promising, for the rest I vote 'no-go.'
- Plans are built on past progress and may lead to some improvement. Need to focus on more promising materials/systems rather than only SWNT. Need to explore the possibility of applying this concept to other types of materials.
- Their proposed future research is considered to be the best one at present stage.
- For the most part, the FY 2008 plans are a logical extension of their work to date. Next year they should give more detail on the nature of their collaborations within and outside the Sorption CoE. A major point of emphasis should be to get some kind of reasonable hydrogen sorption result near ambient temperature.

Strengths and weaknesses

Strengths
- Strong approach and creative design strategies are in place and are providing a fruitful composition space for synthesis.
- Nice to see work devoted to scale-up and improvement in the production process of these materials.
- The general approach is novel and is focused on overcoming most of the technical barriers.
- Interaction with people on the computational side and the measurement side through the CoE activity.
- Their technology for synthesis of nano-structured materials.
- Cross linking possibility could be applied to other carbon based materials.
- This group is a world leader in the synthesis of nanoscale carbon structures.
- Their close proximity to the Yakobson group serves them well.

Weaknesses
- More emphasis should be placed on hydrogen storage property evaluation and the deduction of structure-property relationships toward materials optimization. It is additionally important to evaluate and include the properties of materials which have been synthesized in terms of volumetric capacity, response to cycling, kinetics, and binding energy (i.e. the DOE targeted criterion).
- Li does not perform Kubas binding. It enhances the H_2 binding by charge induced dipoles. A better understanding of the phenomenon is needed.
- The cost barrier was not addressed in this project.
- There are no obvious weaknesses in this project. The overall approaches and capabilities are among the best one will find in any of the hydrogen storage CoEs.

Specific recommendations and additions or deletions to the work scope

- Overall scope of project is aligned. Shift toward property evaluation recommended. Additionally, continued communication between Rice and NREL is recommended in regards to the work on C60 to avoid duplication of research.
- Suggest adding the scale-up issue to project scope.
- Suggest sending some foam materials to MH center to incorporate their result.
- Kubas-type binding proof of concept illustration is recommended for the 2007 work to support a "go" decision
- It's not too early to start thinking about what can be done to get upwards of 10 wt.% H and 100 g/L for carbon-based materials because it will probably take these kinds of material storage levels to meet the 2010 system targets once the balance of system is taken into account. A compensation factor near 2.0 is emanating from systems studies reported in other presentations at this year's Peer Review. If that is out of the question for carbon-based materials, someone should be prepared to “step up and say so”.

Project # ST-06: Metal-doped Carbon Aerogels for Hydrogen Storage

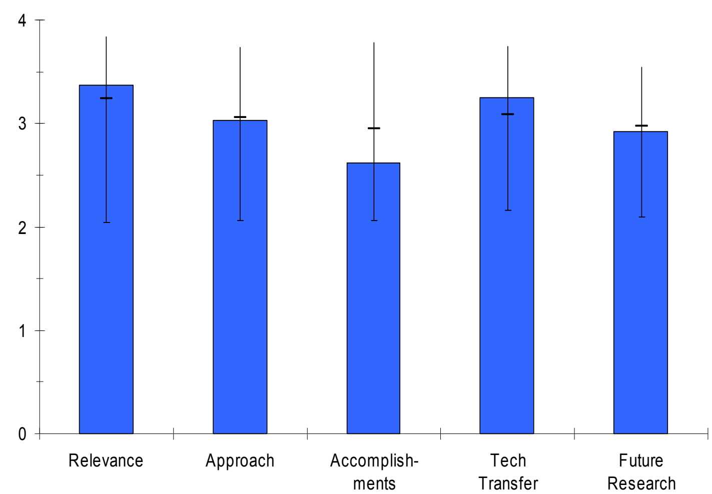
Ted Baumann PI, presenting; Joe Satcher, Co-PI, M. Worsley, J. Herberg, Lawrence Livermore National Laboratory (LLNL)

[Member of the Hydrogen Sorption Center of Excellence]

Brief Summary of Project

Designing new nanostructured carbon-based materials that meet the DOE 2010 system targets for on-board vehicle hydrogen storage of 6 wt.% H_2 is the objective of this LLNL project. Metal-doped carbon aerogels (CAs) will be prepared, characterized and evaluated for their hydrogen storage properties. Mechanisms associated with hydrogen adsorption in these materials will be investigated using advanced nuclear magnetic resonance (NMR) techniques. In 2007, LLNL incorporated dopants, such as boron or metal nanoparticles, into CAs to increase H_2 binding energy (> 10 kJ/mol).

Overall Project Score: 3.0 (6 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.4** for its relevance to DOE objectives.

- Project focus is on low cost, high efficiency storage materials. However, it is unclear why carbon aerogels would provide any performance benefits as compared with other adsorbents.
- Fits well into DOE objectives and President's HFI. Focuses directly on targets and goals of HFCIT multi-year RD&D program plan (MYPP), especially the most important gravimetric and volumetric H-densities. A few comments on cost would have been useful; presumably aerogels can be manufactured at lower cost than some other forms of carbon.
- Carbon aerogels will only have significant hydrogen storage capacity at 77K, and not room temperature. Carbon aerogels will likely not meet the 2010 volumetric storage targets.
- The project is closely related to the DOE Hydrogen Initiative and overall objectives. The design of new CA materials with the flexibility of incorporating dopant is critical to overcome the technical barriers.
- Project is highly relevant to storage targets. Barriers A, C, P addressed.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- One of the advantages was stated to be incorporation of dopants into sol-gel precursors in the stage of synthesis of aerogels, then it was stated that this method would not work because of activation process. If that is the case, there seems to be no advantage versus other carbon materials.
- Controlled aerogels complements other carbon projects. Good porosity control of C-nanostructures. Metal doping seems to be a highly worked area; this work can perhaps complement other DOE carbon project efforts, but project should take care to avoid duplication. Use of controlled C-aerogels as scaffolding for hydrides is an excellent idea, perhaps more valuable than use as an H medium *per se*.
- Trying to further manipulate the porosity morphology in carbon aerogels may have reached the point of diminishing returns.
- The approach is focused on technical barriers and enables surface modification of carbon.
- Pore size distribution can be easily controlled to a certain range with this approach.

- The approach is scalable.
- The cost issue was not addressed in the approach.
- The approach is sound and interesting, definitively worth investigating. Offers an interesting alternative to activated carbons and other nanocarbon materials. Excellent team.
- The barriers identified in 2006 are tackled which led to improved wt.% hydrogen uptake-very good progress!

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.6** based on accomplishments.

- Advantages over other carbon systems have not been demonstrated. In fact storage characteristics were inferior to other known "physical" adsorbents.
- Have demonstrated excellent ability to control aerogel microstructures, pore size, surface area, etc. Room temperature data not yet obtained, but one can probably predict aerogel carbons will not have very useful capacities at ambient temperature. M-doping seems to have only marginal benefit, at least so far at low temperature. Good progress in technical understanding. Progress in H-storage capacities suggest DOE targets will not easily be met with the M-doped, but the idea to use C-aerogel as MH scaffolding may be a much better approach.
- Very good progress on pushing the carbon aerogel hydrogen storage capacities at 77K. Relatively little progress in using metal additives to the aerogel to increase storage capacity.
- Demonstrated good improvement in hydrogen storage, compared to standard carbon aerogel materials.
- The best material achieved is not as good as activated carbon in terms of desired pore size distribution.
- Some improvement of binding energy, still below stated objective. Good storage densities for cryosorption, however the results are similar to activated carbons (minor effect of doping so far).
- Porosity control methodology needs to be focused on more. Hydrogen uptake of 5.3 wt.% due to activation is a good improvement from last year's results.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.3** for technology transfer and collaboration.

- Useful collaborations, at least on paper. Source of collaborative data not always clear in presentation. No NS [neutron scattering?] or NMR results shown. Collaboration with HRL (aerogel scaffolds) is a great plus. It this effort a direct component of the HSCoE?
- Project is seeking out other possible uses for aerogels, such as scaffolding for higher capacity hydrogen storage materials.
- Good collaboration with other groups.
- Need to explore the possibility of using the materials developed in this project for other applications.
- Clear collaborative framework. Good collaboration with others within the DOE program (i.e. HRL).

Question 5: Approach to and relevance of proposed future research

This project was rated **2.9** for proposed future work.

- "Scaffolding" metal hydrides in the framework would not significantly improve basic characteristics of metal hydrides (except kinetics, perhaps). (Refer to earlier work by NREL on SWNTs loaded with hydrides).
- Future work is built on past results and is logical to complete the fundamental understandings of C-aerogels. Further doped- C work may not be very productive toward breaking the technical barriers.
- Expansion of original effort to MH scaffolds seems the most value for a breakthrough (HRL connection).
- Good, but there doesn't seem to be very many avenues identified for improving the storage behavior of the metal additive doped carbon aerogels.
- The plans are built on past progress.
- The PI needs to layout a strategic and realistic approach in choosing the dopants.
- The PI needs to consider how to improve the thermal conductivity of the material.

- Boron work could be interesting. Difficult to see yet how substantial improvements over activated carbons could be achieved. The team is proposing an interesting refocus: scaffolding strategy interesting.
- Path to tune the porosity is not clear and might not be simple; this could be a show stopper for utilization of aerogels as hydrogen storage materials.

Strengths and weaknesses

Strengths
- Use of relatively low-cost materials.
- Is doing work on C-aerogels, a complement to similar work elsewhere on other types of C?
- Offers a potentially low-cost alternative to other carbons, such as nanotubes.
- Offers an important extension to using the aerogels as scaffolds for MH, not as H-storage media themselves.
- Excellent expertise on the aerogels and their synthesis.
- Carbon aerogels can be made with high surface area.
- Carbon aerogels are potentially relatively inexpensive materials.
- The approach is simple and scalable.
- May offer a practical pathway to doping carbon structures (compared to activated carbons).
- Improvement of activation procedure and consequently improved wt.% hydrogen uptake.
- Collaboration with others within the DOE program.

Weaknesses
- Essentially all capacity measurements were done at 77K that may not demonstrate any potential leads towards more practical applications at ambient temperature.
- Like all C adsorbent work, this does not seem like a likely route to reaching DOE 2010 gravimetric and volumetric storage targets.
- At best, undoped or metal-doped aerogel storage will probably require cryogenic containers.
- Carbon aerogels are likely to have relatively low volumetric hydrogen storage capacities.
- Incorporation of effective metal dopants into the aerogels to increase storage capacity appears to be very problematic, and may not be feasible.
- The theoretical limit of this kind of material in terms of hydrogen storage capacity, how it compare to activated carbon and MOFs was not addressed.
- Difficult to imagine how the pure materials will be able to achieve the DOE targets.
- Need to clarify path suggested to enhance and control porosity of the aerogels.

Specific recommendations and additions or deletions to the work scope

- Consider evaluating the spillover effect and capacities at ambient temperature and move on to a go/no-go decision.
- There should be a go/no-go decision point during the next year concerning the viability of using C-aerogels (undoped or doped) as H-storage media.
- Further increase project scope and direction in the direction of using C-aerogels as MH scaffolds.
- None.
- Very interesting and recommend to continue funding.
- Need to clarify path suggested to enhance and control porosity of the aerogels.

Project # ST-07: Enabling Discovery of Materials with a Higher Heat of H_2 Adsorption

Alan Cooper, presenting; H. Cheng, M. Foo, J. Zielinski, C. Coe, G. Pez, Air Products & Chemicals, Inc.

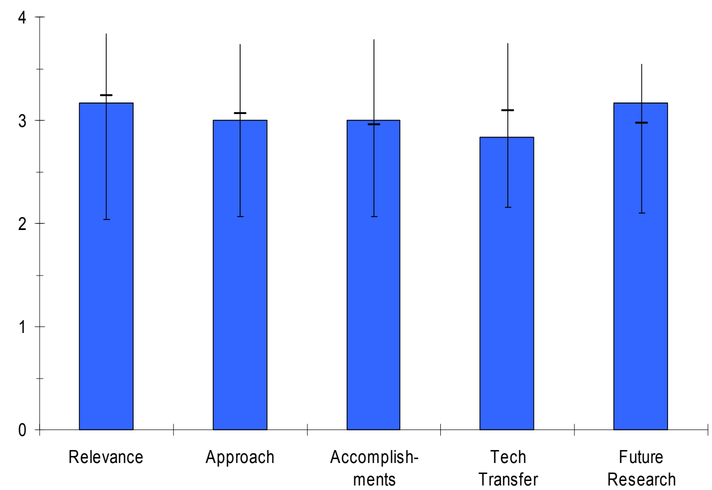
[Member of the Hydrogen Sorption Center of Excellence]

Brief Summary of Project

The objectives of this project are to:
- Develop enabling technologies for H_2 storage materials development;
  - o Accurate, predictive computational methodologies for new materials discovery and mechanistic understanding,
  - o Characterization tools for accurate H_2 storage measurements,
- Develop and test of new materials with high H_2 storage density and appropriate enthalpy of hydrogen adsorption.

The overall goal of this project is reversible adsorption of hydrogen at near-ambient temperatures at densities that will enable meeting the 2010 DOE system-level targets for hydrogen storage.

Overall Project Score: 3.0 (6 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.2** for its relevance to DOE objectives.

- Aligned and relevant to the DOE objectives. Even though not critical, still instrumental for the success of the Sorption CoE projects. Provides data and guidance on the limitations and performance improvement possibilities of carbon based materials.
- Project fits within President's Hydrogen Fuel Initiative. Project generally directed toward HFCIT MYPP, mainly gravimetric H-density. Other target parameters (e.g. volumetric H-density) not discussed much.
- The project involves a combined theoretical and experimental study where theory predicts promising materials and experiment develops and tests these new materials.
- The work is too preliminary to assess relevance with respect to the DOE goals for storage.
- High degree of relevance to guide the development of new materials that could meet the storage targets and to the understanding of physical processes needed.
- Understanding the hydrogen spillover mechanism could lead to the discovery of improved hydrogen storage materials. This is a key mechanism to understand for almost all adsorbent based materials.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- Well-thought approach. It involves predictive computational modeling for screening materials with respect to their hydrogen storage capacity and adsorption energy prior to synthesizing and testing them. Valuable contribution to the improvement of accuracy of adsorption measurements - this is of particular importance to the microporous materials.
- Part of project's approach is to support various HSCoE efforts with theoretical (computational) aspects of H-spillover. That is valuable to help decide if spillover has any hope of overcoming weight-volume barriers. PI notes the advantage of close connections between calculation activities and experimental. Project activities are rather diverse and scattered, but should contribute in a useful manner to the H-program. Project's emphasis on identifying new and different materials is very important.

- The theoretical methods and software used are standard and the energetics are computed efficiently. However, the results are not well integrated with experiments and other research.
- Several different systems have been considered, either experimentally or theoretically, but it is not clear what the overall program direction is.
- Very interesting results obtained using ab-initio approach. Some validation is shown, however should be complemented by experimental work by partner organization.
- Using appropriate modeling tools to understand the binding energy discrepancies in the various stages of the spillover mechanism - an adequate explanation must be provided in order to give credence to this mechanism. Modeling will need to be followed up with real analytical tools to observe and validate the hypothesis put forth.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- Sound progress and satisfactory degree of achievement with respect to objectives and original planning. Identification of promising storage materials that could demonstrate practical hydrogen adsorption enthalpies at high hydrogen loadings and could be synthesized in the lab. First insights into the hydrogen spillover mechanism.
- A good and more complete story on the mechanism of hydrogen spillover has been accomplished. It seems, at least relative to carbon and Li-intercalated C, that the calculational results are rather negative relative to meeting MYPP RD&D targets. For example, it appears that it will promote strong C-H bonds that may require excessive temperatures to break. It is not clear what the PI recommends for the future of other DOE projects involving spillover. Is there hope of reaching DOE targets at room temperature? The prediction of a new material (N-F-graphite) gives great hope of overcoming the weight barriers. This is a valuable result that should be experimentally confirmed ASAP. It is hard to judge this project against its own schedule and milestones, which were not given in the presentation.
- Theory has identified possible synthetic routes to produce porous nitrogen-based graphite intercalation complexes. There is no clear demonstration that the theoretical prediction has resulted in the discovery of new materials.
- The technical progress was not clearly summarized in the presentation. Only a few systems were examined using modeling tools but there was not much to report on new material development and testing.
- Shows possible pathways to achieve the DOE storage targets. Good contribution to understanding the mechanisms of spillover and related phenomena. Proposes new promising materials for sorption based storage that could meet the DOE targets. Proposes bridging/storing class of materials to improve spillover mechanism.
- Good explanations of Pt clusters provided and how large clusters must be in order to propagate the spillover mechanism. PI should offer some insight as to how the spillover mechanism is initiated (not just propagated). Can surface defects provide the initiation sites?

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.8** for technology transfer and collaboration.

- Already well connected to a number of CoE members involved in the same research field and in anticipation of enhancing these collaborations and establishing interactions with others.
- PI lists NREL, ORNL and Penn State as collaborators, but does not really define their roles. PI lists possible future collaborations, but does not really define their roles. Collaborations seem to be mostly within the HSCoE.
- The project is not well coordinated with similar work being carried out at other institutions modeling spillover mechanism.
- It is not clear what the next step will be in the program if the nitrogen-doped carbon materials are not effective. It is not clear how this work has enabled others in the CoE.
- Degree of input of other partners seems low or has not been clearly expressed in the presentation. The project would benefit from collaborations with other program funded projects.
- Air Products is always limited in their collaboration. However, they have the appropriate level of in-house expertise to conduct such work.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.2** for proposed future work.

- Sound & targeted future planning building on recent progress and moving a step forward.
- Future work is based on past results and aimed toward technical barriers. Work on N-F-graphite and computational identification of new materials is good. Spillover work seems about finished. It would have been useful to clearly state the PI's conclusion from the calculations – does spillover offer much hope for developing a C-based material that can meet DOE targets for 2010 or beyond?
- Complete synthesis of graphitic carbon materials with nitrogen doping and using these materials to generate fluoride intercalation will be very worthwhile project.
- The future work has limited scope and there is not clear pathway forward if the next system, the nitrogen-doped graphite, does not have success.
- Excellent progress, logical next steps.
- They need to clarify if they will pursue some of these fluorinated compounds and to what extent.

Strengths and weaknesses

Strengths
- Lengthy experience and competence in the field.
- Strong collaborations pulling expertise and forces within the CoE, particularly in the field of synthesis.
- Project has good people with good new ideas and excellent technical and industrial experience.
- Project aims at identifying new and very different materials through calculational modeling. Yes, other projects are also doing that; but this project's methods seem somewhat different.
- Experiment is aiming at synthesizing theoretically predicted materials.
- Difficult modeling work was completed.
- Interesting quantum chemistry study of the spillover mechanism.
- Proposes strategies to enhance the effect.
- Exciting results for carbon-nitrogen-fluorine structure (strong binding physisorption).
- Air Products is an industrial company that is motivated to produce hydrogen storage materials for their own gain. They have a good understanding of automotive and industrial requirements and choose their research directions wisely based on real-world economics and knowledge.

Weaknesses
- Validity and reliability of the ab-initio molecular dynamics simulations presented.
- Identification of limitations/downsides of proposed methodologies – for instance difficulty in removing the THF solvent in the process proposed for the Li-building carbon materials.
- Volumetric and other DOE targets hardly mentioned. In addition to calculating gravimetric H-densities, we should see some simple calculations on volumetric densities. Can this general volume barrier problem be overcome with sorption materials based on carbon?
- This reviewer would like to see hydrogen expressed in wt.% rather than cc/g (Li-doped SWNT slide).
- Collaborations are not clearly defined.
- Some of the work is not very relevant to the program goal. For example, studies of hydrogen interaction with free Pt clusters does not elucidate spillover mechanism as it is the supported metal cluster that is important.
- The project would benefit from a clearer program plan, both with respect to material development and for enabling interactions with other CoE participants.
- Lack of experimental work.
- Limited validation.
- Clearly needs experimental feedback.

Specific recommendations and additions or deletions to the work scope

- Benchmark computational modeling data with experimental data; check their validity.
- Consider accelerating the material synthesis and testing program.

- A general comment – there is a strong need to reach an agreement on how storage capacity data are presented – excess, total or absolute hydrogen uptake?
- Phase out spillover work and increase efforts on experimental confirmation of identified new materials.
- Focus on new N-F-graphite. It seems to offer greater hope for a "breakthrough", as suggested by the preliminary calculations of ΔH = -20.2 kJ/mol and wt.% = 7.4. Look for new and different materials.
- Efforts should be more coordinated between theory and experiment relevant to the program goals and between various groups working on similar problems.
- Collaboration with Yakobson and Hauge from Rice strongly suggested in order to coordinate theoretical activities on spillover.

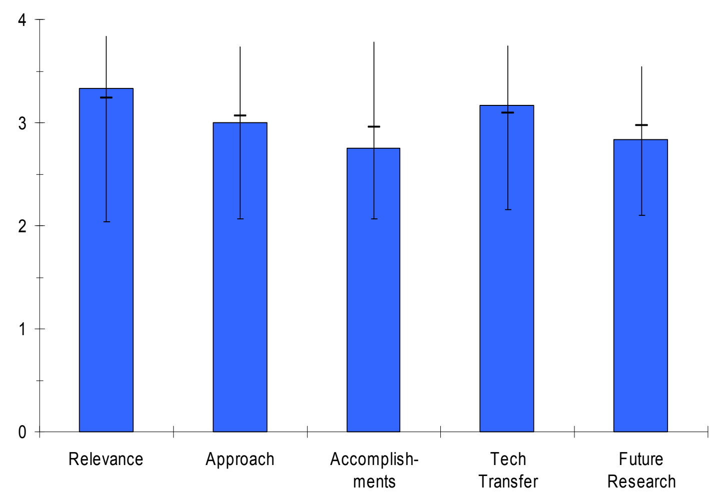
Project # ST-08: Advanced Boron and Metal Loaded High Porosity Carbons
Mike Chung, Presenting; Peter Eklund, Hank Foley, Vincent Crespi, Co-PIs, Pennsylvania State University

[Member of the Hydrogen Sorption Center of Excellence]

Brief Summary of Project

The overall objective of this project is to develop advanced hydrogen physi/chemisorption materials that are reversible, have high gravimetric and volumetric capacity and favorable thermodynamics. The goal is to achieve reversible storage of ~6 wt.% at 200K, 100 atm by 2008. High specific surface area (SSA) carbons are the focus of this work. The carbon framework will be chemically modified for enhanced H_2 binding energy. Boron will be substituted to enhance the binding energy of hydrogen. Boron is a light element and the only one known to substitute in the sp^2 framework without serious structural distortions.

Overall Project Score: 3.0 (6 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

- The effort of chemical modification of carbon to adjust H_2 binding energy is good and relevant for efficient storage. Too much focus on achieving good capacity numbers at cryogenic temperature which has little relevance to potential commercial applications for on-board storage.
- There is some doubt that this approach can meet the 2010 targets, even at 77K.
- The project is closely related to DOE HFI and overall objectives. Synthesizing the B/C materials with desired B content and SSA is critical in overcoming the barriers.
- The project is highly relevant to the DOE RD&D objectives. Barriers A and P have been addressed in the presentation.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- Increasing boron content and enhancing SSA is the right approach for doped carbons. However, more studies should be done at temperatures other than cryogenic.
- There needs to be more emphasis on ways to incorporate higher binding energy species into the B-C structures. What is the strategy for incorporation of these species?
- Theory guided experimental design is a good approach. The experimental approach is scalable. The PI needs to address how to control the structure and content of the final product in the approach.
- The approach to meet the project objectives is sound.
- Molecular reaction and electric arc appear to be brute force approaches to synthesis and do not show any path forward to controlling the boron concentration on an atomic scale. Polymeric precursor route to boron modified carbon appears to be only path to control boron concentration. There are no systematic experiments planned or discussed with respect to the polymeric precursor route. There needs to be a controlled set of experiments to evaluate boron concentration effects as well as surface area. There needs to be some determination of the theoretical limits of boron exchange in the graphene layers.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.8** based on accomplishments.

- Still, best boron-doped carbon demonstrates significant disadvantages in capacity versus other materials such as MOF's and high SSA carbons. There is a good correlation of boron content and "specific" capacity - 5.7% boron gives ~ 330 m^2 per wt.% capacity, and 8% boron gives ~ 244 m% per wt.% capacity (compare MOF ~ 840 m^2/g and commercial carbon ~500 m^2 per wt.% capacity). Assuming trend continues with the increase of boron, a weight capacity of 10% could be feasible if SSA increased up to 1700 m^2/g. It is challenging but not unrealistic, however, this would be at cryogenic temperature. Progress isn't enough to anticipate meeting the targets for storing hydrogen at ambient temperature.
- Boron additions do show some level of improved hydrogen adsorption, but not enough to get “excited” about. Multiple synthesis techniques for incorporating boron into the carbon structures have been developed. The high temperature synthesis of boron-carbon nanoparticles is interesting.
- Demonstrated certain progress towards the target. Room temperature hydrogen uptake at less than 1 wt.% should not be used as a measure for accomplishment. The PI needs to specify the size of error bar for 0.5 wt.% hydrogen uptake.
- Substitution of carbon material with B, C, Al etc., considered to be one of effective techniques. However their strategy and result do not suggest certain achievement of hydrogen capacity over 6 or 9 wt.% .
- Promising storage densities have been achieved experimentally (taking into account the specific surface). Lower end of H_2 binding energy of project objective has been achieved. Interesting theoretical work.
- The technical accomplishments are minimal. Only the chemical synthesis method has generated any material with substantial boron levels. The hydrogen storage is not better than that of any other carbon material. The boron additions increased the binding energy and to some degree the hydrogen storage capacity. At what point is the binding energy too high for this to be a useful material?

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.2** for technology transfer and collaboration.

- List of partners is very limited, however, membership in the CoE should help enhance collaborations.
- There is good collaboration to characterize the materials being produced.
- Certain coordination within the CoE exists. Need more collaboration with other groups.
- Good Penn State team integration, not as clear from the presentation what the contribution of the other partners were.
- Collaborators were listed but there was no mention of how the team interacts with the CoE or the collaborators. Detail is lacking.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.8** for proposed future work.

- Proposed future research is good, but there appear to be no radically new approaches proposed to increase the hydrogen storage levels from where they are now, except to pursue the addition of selected metal atoms to the boron-carbon structures.
- Plans are built on the past progress and sound good. Need to layout a specific pathway to execute the plans.
- It is expected that they find a pathway to improvement of hydrogen capacity over 6 or 9 wt.% in system by increase of heat of adsorption.
- Logical next steps are considered.
- The future work lacked a detailed explanation of how they are to achieve their results. The future work was to achieve a certain boron level by a certain date or a certain storage capacity by a certain date. The details of how they plan to get to these levels or if these levels are possible were lacking.

Strengths and weaknesses

Strengths
- Good lead in terms of increasing "specific" capacity (SSA per wt.% storage).
- Very good scientific approach to explore boron additions to carbon to improve hydrogen storage.
- Multiple synthesis avenues are being pursued.
- Hydrogen storage reversibility should be good for these types of materials.
- Theory guided experimental design is very effective.
- The approach is scalable.
- Assuming that the specific surface can be scaled up to 2800 m^2/g then a storage density of about 11% could be achieved for cryosorption (may meet the 2010 DOE storage density system target).
- Net increase of H binding energy.
- Polymer precursor route to boron modification of the graphene sheets is interesting.

Weaknesses
- Low probability of success if storage at ambient temperature is considered instead of cryogenic.
- It is not clear that the boron addition approach will be sufficient to achieve 2010 storage targets.
- Lack of specific technically feasible pathway to execute the plans.
- Room temperature adsorption remains low (cryosorption needed).
- The materials produced need to be more fully characterized to determine where the boron resides and how it impacts the crystal structure. Boron NMR would be the first step as would TEM.
- Systematic studies of boron concentration effects need to be implemented to determine if there is a critical boron concentration.
- Material produced to date is of low surface area. Surface area increased by CO_2 activation. PI needs to understand that boron additions make the carbon structure more stable to activation and more difficult to increase the surface area. This looks like a “dead-end” approach.

Specific recommendations and additions or deletions to the work scope

- Include other elements as dopants in the search. Boron will most likely to help achieve targets at 77K but not at 25°C.
- The study of non-stoichiometric carbon-rich B4C might prove interesting.
- Determine what is the desired structure (pore size, BET, etc.) and feasible B/C ratio. Determine whether there is a structure change compared to pure carbon materials.
- Eliminate electric arc and molecular reaction synthesis routes as they do not appear to demonstrate to control boron concentration.
- Some in depth characterization of the structure with boron is needed.
- There are no systematic experiments planned or discussed with respect to the polymeric precursor route. There needs to be a controlled set of experiments to evaluate boron concentration effects as well as surface area.
- The materials produced need to be more fully characterized to determine where the boron resides and how it impacts the crystal structure. Boron NMR would be the first step as would TEM.
- Systematic studies of boron concentration effects need to be implemented to determine if there is a critical boron concentration.

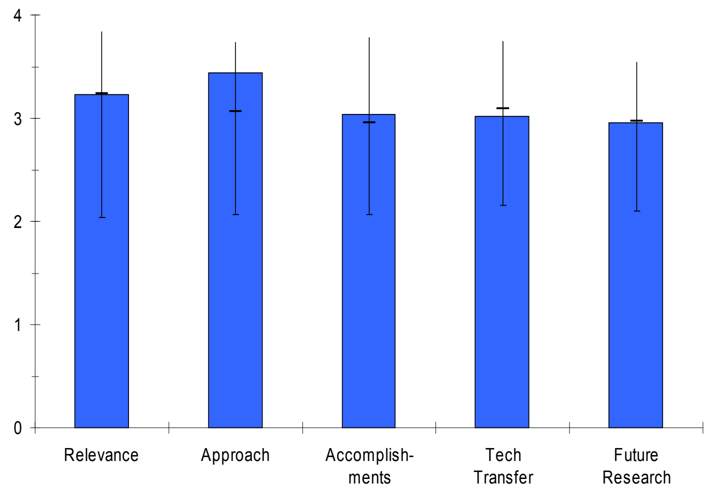
Project # ST-09: Carbide-Derived Carbons with Tunable Porosity Optimized for Hydrogen Storage
Jack Fischer, presenting, University of Pennsylvania; Yury Gogotsi, Co-PI, Drexel University; Taner Yildirim, Co-PI, NIST

[NOTE: This project is not part of the Centers of Excellence; it is an independent project.]

Brief Summary of Project

The objectives of this project are to:
- Develop and demonstrate efficient, durable and reversible hydrogen storage in carbide-derived carbons (CDC) with tunable nanoporosity (2004-2005).
- Determine the optimum pore size for hydrogen storage using experiment and theory (2005-2006).
- Identify post-processing strategies and catalytic additives which maximize the performance of CDC-based hydrogen storage materials, using experiment and theory (2006-2007).
- Finalize the design of a CDC-based H_2 storage material that meets 2010 DOE performance targets and commercialize it (2007-2008).

Overall Project Score: 3.1 (6 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.2** for its relevance to DOE objectives.

- Project focus seems generally aligned with DOE objectives.
- The project aims to develop durable, efficient, and reversible hydrogen storage using carbide-derived carbon with tunable porosity.
- Clear relevance. Barriers A, F, Q addressed in the presentation.
- Directly addresses one approach to materials-based hydrogen storage.
- The stated objective is to develop a system that will satisfy 2010 goals and commercialize it (by 2008). It is not at all clear how the PI will do this (either achieving the 2010 goals, nor commercialization). The specifically tailored pore-sizes could be useful for a variety of purposes; however, it is not clear that changing the pore size will get this idea to room temperature storage (much less a 6 wt.% system at room temperature).
- Project generally supports DOE goals. However, the pathway to achieving the gravimetric and volumetric goals at non-cryogenic temperatures is unclear.
- There may be inherent limitations in capacity and binding energy that could limit reaching goals.

Question 2: Approach to performing the research and development

This project was rated **3.4** on its approach.

- A variety of purification/activation and chemical modification studies have been performed and shown to be effective for tuning the pore size distribution and surface areas of these materials. Fundamental understanding of the structure and hydrogen binding would help to guide and understand research. Additionally it is important to determine the theoretical upper limits for gravimetric/volumetric capacity for these materials?
- This is a unique and interesting approach for fabricating nanostructures with controlled pore size. The ability to tailor the pore size is a promising way to synthesize and test sorption materials with controllable sorption properties. It is highly questionable as to whether these materials will be effective adsorption media at non-cryogenic temperatures. The strong synthesis and characterization effort is enabling rapid progress toward

establishing the efficacy of this approach for enhanced hydrogen sorption. There is good support from theory to describe how changes in structural properties affect sorption behavior. This will continue to be important for understanding and optimizing sorption enhancement by doping and chemical modification.

- Approach involves creation of pore structures, optimization of the size and shape of the pore, and developing techniques for purification and doping.
- Approach ("designer pore structure") is sound and interesting. Nanodiamond studies were an excellent idea to qualify surface modification strategies.
- Unique approach in tailoring pore size distribution to enhance hydrogen uptake by starting with carbide as a precursor. Emphasis on post-processing strategies to enhance hydrogen capacity has yielded improvements in hydrogen capacity. Should increase efforts toward increasing the hydrogen binding energy. Use of macroscopic configurations (e.g., rolling peels, pellets) excellent approach to enhancing volume density.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- Post-treatment purification of samples using NH_3 or H_2 gas was used for removal of Cl-based byproducts. While necessary, the purity of the effluent H_2 gas needs to be examined. That is, what is the remaining amount of trapped Cl_2 gas ("<1 wt.%" needs to be quantified further)? Does annealing under NH_3 result in trapped/bound/adsorbed NH_3 which would be released? It is good that strategies for improving volumetric capacity are being considered and evaluated. A great deal of progress on gravimetric capacity since 2006 has been demonstrated. Cycling/reversibility studies for these materials are necessary to demonstrate that the chemical (dopants/surface treatments) and structural (pore size/surface area) integrity (and thus properties) are maintained over multiple cycles.
- The accomplishments look scientifically promising, but don't show a real pathway towards improving the technology, or progressing towards DOE targets. Surface chemical modification (to increase binding) results look like a promising avenue to pursue. Li doping studies do not look like a promising approach. Not clear how modeling studies have really significantly taught anything new beyond what was already known from NREL studies.
- Excellent progress on synthesis of a wide range of CDCs with different pore characteristics. Impressive results on enhanced adsorption at 77K. Chemical modification of pore surfaces and synthesis of doped material are promising approaches to achieving improved sorption performance. Control of reaction with Li to achieve high coverage without agglomeration is likely to be problematic. Are theory/modeling predictions available that show which pore size and pore size distribution would be optimum? If so, the project should rapidly focus on those conditions for testing/validation.
- Purification by removing elements that block access to the pores. Chemical modification of the interior pore surface to increase binding. Doping with metal atoms to increase Kubas binding.
- Optimization of pore size distribution and specific surface. Li-doped disappointing at moderate pressures (Li clustering reducing accessible pore volume?) Challenges well identified. Ti dispersion in pores not achieved. Enhancement of the volumetric capacity through compression has been achieved.
- Important results achieved on volume density by compressing powders. Good progress on tuning porosity and cleaning materials, but most of this work was from last year? Major result this year was using ammonia in post process purification treatment. Still limited on volume and weight capacities. Needs further work and accomplishments towards enhancing hydrogen binding energies in these materials to raise the operating temperature. No measurements shown above 77K.
- Although good progress has been made to date, significant improvements in storage densities and binding energies will be needed to meet DOE targets.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- Good collaboration between experimentalists and theorists within the independent project. Recommend initiating interactions with investigators in the HSCoE (there's common ground between this project and the HSCoE activities; both groups could benefit from these interactions). There may also be some good

opportunities for collaborations with MHCoE researchers on the use of these materials as support structures for enhancing the metal hydride reaction kinetics.
- The PI is interacting with theorists to achieve a fundamental understanding of the hydrogen binding to metal doped pores.
- Collaborations and role clearly discussed.
- Some collaborators in specific technical areas. Some leveraging with BES funded activities.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- Future goals such as increasing the heat of adsorption (toward more ambient temperature storage) are valuable; however, it was not clear what the approaches are. As mentioned above, cycling and hydrogen purity studies are important as well as a continued focus on increasing volumetric densities.
- The proposed future research is focused in the right direction (increasing binding, moving towards room temperature adsorption, etc.), but seems a bit unimaginative. It is not clear that the proposed theoretical work will really help move the project forward (particularly in the last year of the project).
- Good science-based approach to optimizing sorption properties is planned. It is important to consider methods for preparing more reactive sites for metal incorporation; however, no specific plans were outlined. Recommend quantification of hydrogen confinement capacity as a function of temperature (e.g. 77K to ~50 deg C)
- Exploit metal-hydrogen reaction to increase hydrogen binding.
- Clear strategy to move forward. Looking forward to the results on the pore structure (proposed neutron scattering experiments and use of reverse MC simulations)
- FY 08 plans very ambitious. Not clear if all could be accomplished. Right direction for some of the FY 08 activities - increasing binding energy and continuing with improving volumetric density.

Strengths and weaknesses

Strengths
- Vast experimental space to investigate and tune materials properties (i.e. numerous activation, purification, doping, and surface modifications being explored).
- Demonstrated control over pore size and surface area properties using above methods.
- Novel approach for preparing unique sorption materials with controllable pore characteristics.
- Strong R&D team comprising both theorists and experimentalists.
- Good possibilities for expanding effort by collaboration with CoEs and other independent projects.
- Knowledge guided approach for optimizing pore size and metal doping.
- Ability to optimize the pore size distribution is demonstrated.
- Substantial enhancement of the isosteric heat of adsorption with respect to conventional carbon structures.
- Designer pore size distribution is an appealing strategy.
- Good approach of forming compressed structures to increase volume densities of these relatively low density materials that might be applicable to other types of adsorption materials.

Weaknesses
- It is not clear that a rational materials design approach has been developed. That is, the effects of the reactants (metal identity) and sample treatments (activation, purification, and surface modifications) on the resulting product structure need to be understood. This would clarify the path forward toward improved properties.
- Operation at non-cryogenic temperatures is a critical issue and potential showstopper for this approach. This should receive greater emphasis.
- The theoretical work is not relevant to project goals. Using $C_2HA(Ti)_2$ to understand what happens in Ti doped pores is inappropriate.
- Doping these structures appears problematic.
- Needs higher temperature capacity measurements on doped samples.
- Not clear how modeling works into experimental work.

Specific recommendations and additions or deletions to the work scope

- The challenge of modeling these amorphous, non-periodic systems was acknowledged and potential options introduced. It would beneficial to try to incorporate some theoretical aspects (identification of best dopant or surface functionalities) to better guide their research.
- Experiments which investigate hydrogen gas purity and reversibility should be incorporated.
- None.
- The PI should be more critical of theoretical models and encourage calculations that are appropriate for the experimental morphology. Efforts should be made to determine if metal atoms inside pores cluster or remain isolated.

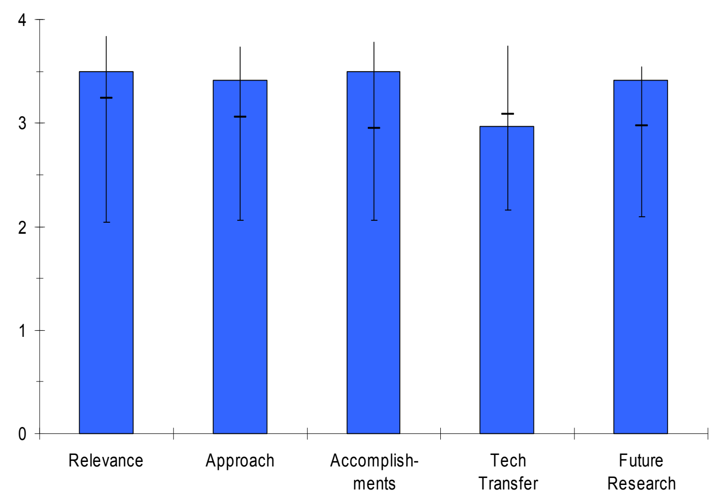
Project # ST-10: Hydrogen Storage in Metal-Organic Frameworks
Omar Yaghi; University of California, Los Angeles (UCLA)

[NOTE: This project is not part of the Centers of Excellence; it is an independent project.]

Brief Summary of Project

The overall objective of this project is to develop strategies for achieving metal-organic frameworks (MOFs) that have increased uptake at higher temperature. This is being done by utilizing new concepts for increased surface area, implementing strategies for higher adsorption energy, and developing strategies for increased hydrogen density. Progress in 2007 included:
1. Tuning porosity led to tripling of hydrogen uptake in MOFs (excess 7.5% wt., absolute 12% wt.);
2. The 35 grams H_2/L achieved in MOF-177, indicates that dead volume is not a major issue for MOFs;
3. MOFs exhibit fast kinetics (1-3 minutes for charging and discharging);
4. MOF material porosity and uptake are stable to charge/discharge cycling;
5. Cubic meter scale of useful MOFs is now being developed by BASF.

Overall Project Score: 3.4 (6 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

- Research directions followed are generally aligned to program's objectives and support the Hydrogen vision.
- High surface area materials are an important part of the DOE storage objectives and this program is addressing this issue.
- Project is well-directed toward objectives of President's Hydrogen Fuel Initiative. Project focused on DOE objectives and HFCIT RD&D Plan (i.e. MYPP). Project looks closely at both gravimetric and volumetric targets, as well as kinetics.
- The project involves designing the porosity of metal organic frameworks and doping with metal atoms as well as impregnating with polymers to increase the binding energy of hydrogen. Theoretical calculations provide input regarding the metal atoms to be doped.
- Work is directly related to the development of adsorbent materials for hydrogen storage.
- This project brings the concept of reticular coordination chemistry into the DOE Hydrogen Initiative. While it is not likely that metal-organic frameworks (MOFs) in their present state of discovery will meet hydrogen storage targets, the extended study of the first generation of MOFs has stimulated much research into reticular chemistry. The possibility that a reticular structure could meet the storage requirements deserves exploration.

Question 2: Approach to performing the research and development

This project was rated **3.4** on its approach.

- Well-thought, reasonable, systematic approach profiting from the PI's lengthy experience in the field.
- The approach has been focused primarily on 77K sorption condition despite emphasis by reviewers last year to work on room temperature [RT] materials. Some of the proposed approaches towards RT sorption such as Li-

insertion (as shown in the sorption CoE) have been tested with limited success. Need to look at the bridging/spillover phenomenon as developed by R. Yang.
- This effort is well-focused on a large and versatile family of high-surface sorption materials, MOFs and related structures. It is systematically looking at a large variety of MOFs relative to technical barriers. Project aimed at understanding and modifying structures for maximum hydrogen storage capacities with minimum dead volume. This is an important and needed feasibility test for MOFs. Good systematic thinking.
- The PI uses novel chemistry to design materials with different pore sizes and modifying the chemistry of the pores through doping. Fundamental understanding of the science is sought from theoretical collaboration.
- These structures have demonstrated the highest hydrogen capacity of adsorption materials. Has a plan for improving volume and weight densities, as well as increasing hydrogen binding energy - interpenetrating structures, maximizing surface area while reducing large volume, impregnation, etc. New collaboration established with Goddard for theoretical modeling.
- The approach involves the synthesis/construction of strongly bonded, stable, molecular frameworks with controlled pore architectures, dimensionalities, and hydrogen sorption properties. Measurements of the hydrogen uptake and release properties of said molecular frameworks are made routinely. Studies of open metal incorporation, interpenetration effects, combination of MOFs with other framework-like media, and metal atom impregnation are underway. Stability studies are also done as appropriate.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.5** based on accomplishments.

- A very significant step forward. Demonstrated reproducibility of hydrogen adsorption experiments and independent verification of the saturation hydrogen uptake in MOF-177. Proposed a benchmark adsorber: MOF-177 in view of its well-known structure and hydrogen uptake performance. Equally exciting are the possibilities opened by the large free volume in interpenetrating networks – could these hold the secret to a storage solution?
- No significant progress has been made on room temperature sorption materials. The results are not significantly different from what was presented in 2006.
- PI and many coworkers have looked at a large number of materials via theory and experiment. Group has shown up to 7.5 wt.% and 30+ g/L capacity at 77K, i.e., a fair fraction of the DOE system targets. Of course, systems must accommodate reductions from the materials' properties. Group appears to have got a good start on cataloging MOF possibilities in a relatively short time and reasonable cost. Good reversible absorption/ desorption kinetics demonstrated. In summary, good progress has been made against the technical barriers.
- 7.5 wt.% reversible hydrogen storage is achieved at 77K. The synthesized materials exhibit fast kinetics and stability. Efforts are made to scale up production.
- Major effort this year towards interpenetrating structures (IRMOF-62 ~7 wt.%). Increased capacity by opening up metal sites. Still relatively low volume density of these materials relative to e.g., hydrides. Still relatively low hydrogen binding energies with poor room temperature uptake. Soft chemisorption covalent framework studied but only preliminary results. No evidence of high capacity with increased binding energy. Binding energies still remain low in the materials to date.
- The PI has a large group and is broadly funded by several agencies. In future presentations, a slide showing exactly what was done for the project under review would help the reviewer to properly evaluate this metric. Assuming the information on Slide 67 is in fact what was done specifically on the project under review, the progress has been very good. Absolute hydrogen uptake levels at 77 K are now in the range needed to meet system targets for hydrogen storage. The kinetics at 77 K are very good. However, getting reticular frameworks to function effectively and meet targets at ambient temperature is still not achieved.
- The stability results, particularly in aggressive media for some selected structures are impressive.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- Strong interaction and significant technology transfer appears to take place with BASF. However the degree of collaboration with other carbon researchers and institutes is not clear; neither is the link with the Sorption CoE (still important even though the project is outside the CoE).
- Work on MOFs fits well in the R&D roadmap. There are no fixed partners and very limited information on future partners and their roles in the effort.
- The PI collaborates effectively with theorists and is willing to lend expertise and advice to others working on MOFs and COFs.
- Limited collaborations. New collaboration for theoretical modeling. Has collaborated with SwRI on MOF-177 validation and additional testing.
- This project is not part of the Hydrogen Sorption CoE and it is not clear why that is. Other than the Goddard collaboration and the outside testing of a few MOFs, the effort of this project seems to be a “closed shop” operation.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.4** for proposed future work.

- Future research plan builds on current experience and it is appropriately drawn for further progressing towards reaching the objectives.
- The pathway to room temperature sorption materials is not clear.
- PI shows an ambitious and well-considered list of future materials and ideas. Future work built on past results and aimed and weight and target volumes.
- Future work is aimed at increased binding energy for room temperature applications by metal doping, and impregnating with polymers. Testing of new materials (ZIFs and COFs) is likely to enhance the chances of finding suitable materials.
- One senses that the PI has a firm plan for the future that won't be “budged” by recommendations from a reviewer. Nonetheless, getting the reticular structures and/or hybrid structures to meet hydrogen storage target levels at ambient temperature must be the primary future direction for this particular project within the larger Yaghi program. Working on frameworks that might have higher hydrogen absorption energies seems to be essential for this project. The lithium addition and polymer impregnation studies look like good avenues to pursue as well.

Strengths and weaknesses

Strengths
- The PI's and his co-workers’ high caliber expertise in the field.
- Strong background in developing novel materials with very high SSA.
- There is a large and fascinating spectrum of MOFs (and related materials) to look at.
- PI, support and students have very high expertise and potential to fully explore these potentially important materials.
- The project is innovative and the PI is always searching for materials with better performance.
- Very innovative work with large group having good success in synthesizing novel structures.
- Hydrogen program likely benefits from leveraging of resources that the group obtains from other sources.
- A highly leveraged project spearheaded by a determined PI.
- An approach that offers many interesting possibilities for future developments in nanoporous material development.

Weaknesses
- Reproducing this high performance under workable conditions, suitable for transport applications.
- Interaction with carbon research community.
- Scalability?
- Lack of progress in room temperature sorption materials.

- It is uncomfortably apparent that this family of materials may never be practical at room temperature. That is they seem to offer no obvious advantages over other high-surface-area media, except perhaps volume. To be fair, PI expressed some hope for 4-5 wt.% H for Li- or Ti-doped MOFs.
- Focus should be given to keeping the open metal sites from reacting with anything but hydrogen.
- The project might benefit from more interaction and collaboration (where appropriate) with other PIs (e.g., other modelers/theorists, HSCoE PIs).
- The absence of a meaningful interaction with the Hydrogen Sorption CoE seems to be a drawback. Better coordination might help to focus the project on the specific needs of the larger HFCIT program.
- Presentation set of slides are too long and don't follow guidelines.

Specific recommendations and additions or deletions to the work scope

- Enhance interaction and collaboration with the carbon research community and liaise with Sorption CoE.
- Examine the effect of hydrogen impurities on the reversibility, kinetics, durability.
- Investigate MOFs that could have open metal sites and are at the same time interpenetrable.
- This project has delivered excellent results with developing very high SSA materials. However, it has failed to translate this property into useful hydrogen storage materials.
- It is recommended to focus the remaining time and resources to address the room temperature sorption.
- Consider adding collaborative partners.
- Are there possibilities of interest from industry?
- Doping with transition metal atoms should be aggressively explored.
- The work on this particular project should be more narrowly focused to strictly meet the needs of the Hydrogen Initiative.

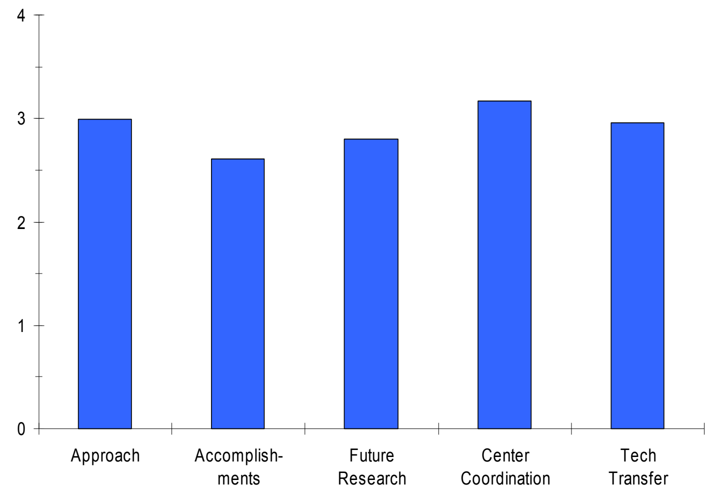
Project # ST-14: DOE Metal Hydride CoE Overview
Lennie Klebanoff, Director; Jay Keller, Co-Director, Sandia National Laboratory (SNL)-Livermore CA

[NOTE: This presentation was to evaluate the entire Metal Hydride Center of Excellence as a whole. A separate review form was used and can be found in Appendix D**.** Sandia's technical contribution to the center is evaluated in ST-15. **]**

Brief Summary of Project

Sandia National Laboratories is the lead partner in the DOE Metal Hydride Center of Excellence, which is composed of 8 universities, 3 industrial partners and 5 other national/federal laboratories. The center is focused on developing new reversible metal hydride materials capable of achieving at least 6 wt.% system hydrogen capacity, improving kinetics of absorption and desorption and thermodynamic plateau pressures, and improving processing and doping techniques that will lower cost. Current materials under study include destabilized binary hydrides, complex anionic materials, amides/imides, and alane (AlH_3). In addition to new materials discovery, Sandia will work with all center partners in fundamental modeling, materials synthesis and modification, testing of hydrogen storage and delivery characteristics, and engineering science and process development to support and guide the materials discovery efforts.

Overall Project Score: 2.9 (7 Reviews Received)



Question 1: Approach to performing the R&D

This project earned a score of **3.0** for this criterion.

- The center activities and project scopes are sharply focused on the DOE objectives, making it a key contributor to the overall Hydrogen Initiative. The center's approach combines synthesis/experiment, theory, and systems analysis, all vital components of a high-impact collaborative hydrogen storage research effort.
- The CoE and the work plan are well-structured with an effective increased contribution of system-related analysis (Project E).
- The program management and the overall revision process are adequately presented with effective selection of promising materials.
- The milestone management style is well aligned with DOE milestones.
- I like the management structure and approach.
- The general approaches are focused on overcoming the technical barriers.
- A lot of activities are directed to address the regeneration/reversibility issue of the materials.
- The center is well organized and is willing to self down select without pressure from DOE or the tech team. The project and program work is well divided in terms of partner capabilities. The work is directed at appropriate questions, such as higher capacity and lower enthalpy of release, though a clearer plan for fast progress on enthalpy and kinetics might improve the center slightly. Theory is well used to help guide experiment; the feed back to theory is present but might be improved a little.
- Organic down select is organic, so far no need to force a down select but council will step in if needed.
- Technical feasibility of metal hydrides is very limited for on-board storage primarily due to low storage energy efficiency, and therefore, low potential of most of metal hydrides studied by the center to meet the program objectives. Only [just] a few leads may be considered as potentially feasible, such as alane that still requires off-board regeneration.

- The strategic focus of the CoE is not critically described by the Coordinator in relation to the DOE technical barriers.
- The down-selection approach needs more specifications and clarity: no criteria have been presented, even during the discussion.
- There are not clearly justified duplication/overlapping in the theoretical material selection approach: various methods are applied in different CoE projects with no clear comparison and integration among them (Monte Carlo, Combinatorial, First Principles). The Theory Group must better describe the way the methods and the efforts are effectively combined.
- The Management cost share (13%) is not adequately justified by the actions described.
- The overall R&D approach must be more tuned with the application-oriented approach of the DOE Hydrogen Storage Subprogram, instead of the used research-oriented approach.

Question 2: Technical accomplishments and progress toward DOE goals

This project was rated **2.6** on this criterion.

- The progress has been well summarized, showing relevant results in term of scientific (62 publications) and IP (10 patents) production.
- The center has shown certain progress in overcoming barriers.
- Some promising results have been demonstrated.
- Significant progress has been made, but using a fairly large budget 8.2M$. Multi-hotplate device is about "ready to roll," but after a rather long generation cycle. $Ca(BH_4)_2$ work is quite an interesting result, though a lower desorption temperature is required. Getting Mg in aerogel is a nice accomplishment; $LiBH_4$ in aerogel did help kinetics. Alane work is appropriate though not much progress this last year. Tank work analysis is appropriate and may be helpful in future when proven out. Theory work is good, but needs to incorporate multi-step nature of reactions - not average over all steps - as its output.
- It is clear, since the presenter mentioned it several times, that they are focused on the DOE goals and aware of the gaps.
- There has been good progress and research devoted to alane regeneration with several different avenues being concurrently explored. Additionally, the modeling portion (particularly that regarding mixed borohydrides) of this center seems to have really aided in providing promising 'leads' to the experimental projects. It is however, important for the theorists to evaluate the stability and step-by-step decomposition energetics of all compositions (rather than just the reactants to products average). Independent and/or internal cross-validation of experimental measurements between partners is also encouraged.
- No/little progress has been demonstrated in the area of complex metal hydrides, amides/imides and destabilized hydrides. These materials may be considered for a quick no-go decision due to low potential for increasing useable storage capacity.
- The progress has been only partially analyzed with respect to DOE objectives and barriers.
- The presentation gives more emphasis to the progress of materials selection and less to the effective possibility to overcome DOE Program barriers.
- All the accomplished materials are still far away from DOE 2010 targets.
- Lack of a well defined pathway to achieve DOE targets.
- There should be more accomplishment with the $8 million spending.

Question 3: Proposed future research approach and relevance

This project was rated **2.8** for this criterion.

- Future plans are appropriate but a deliberate focus on kinetics, enthalpy, and release temperature might yield a better plan. As mentioned above feedback to theory should be planned to a greater extent.
- The timing for the materials down-selection process is reasonable for the DOE target dates.
- I was pleased to learn the CoE structure is flexible and can be reorganized, as appropriate, based on promising new materials.
- A detailed description of future work was not clearly communicated in the presentation. Continued work on higher-valent borohydrides (and mixtures containing them) is promising. Alane regeneration method work

should also continue to be explored in more detail. More importantly, kinetics seems to be a (the) major barrier in the center and should emphasize or devote resources to this problem. Should clarify more how internal go/no-go decisions are made.
- The future plans are not clearly presented.
- The revision and contingency plans to dynamically modify the CoE activities are not adequately planned.
- Time planning showed in slide 24 seems too slow to well address results and efforts toward the final 2010 target.
- It is suggested to concentrate on materials potentially meeting more DOE technical objectives, extending the analysis also to cost aspects.
- The continuous update of material focus may require plans to involve other participants and/or projects in the CoE R&D effort, but it does not seem to be considered.
- The work plans are built on past progress.
- The down selection criteria were not well defined.

Question 4: Coordination, collaborations and effectiveness of communications within the CoE

This project was rated **3.2** for this criterion.

- Communication between center projects is well coordinated and organized. Examples of cross-project interactions were presented to exemplify this established dialogue. Materials systems appear to be rapidly screened and efficient go/no-go decisions made to focus effort on the most promising materials systems.
- Good collaboration and alignment with partners and DOE milestones.
- The coordination and collaboration is well structured.
- Demonstrated good coordination within CoE.
- The composition of the Coordination groups and projects show well organized exchange of information and expertise, well supported by the Coordinator communication plans.
- Based on the information provided, coordination and collaboration appears to be very good.
- It is not clear how intellectual property (IP) aspects have been regulated to improve faster and more effective collaborations.
- Generally well coordinated internally and externally. Would prefer to see a bit more integration of fast throughput into the overall work of the group. Other subcontracts, say LLNL, or HRL, or the theorists seem to help out team members or share their thrusts and expertise regularly. Integration of combinatorial and theory work would seem appropriate to do. SRNL and Intematix in particular seem rather “close to the vest” on science (not engineering, SRNL is open there).
- The Theory Group may reduce apparent efforts [and] duplication by comparing and optimizing the use of theoretical methods for material selection applied in the different projects.
- Need more collaboration between modeler and experimentalist. Certain experimental restrictions and feedback need to be filtered through the modeling work.
- Collaborations between the project and researchers are not visible for their presentation even it is emphasized in this presentation.
- More close discussion of approach and target discussion is necessary.

Question 5: Collaborations/Technology Transfer Outside the CoE

This project was rated **3.0** for this criterion.

- The Coordination with the other CoEs is conveniently increasing.
- External communication seems good. Greater leverage by use of outside partners might be a way to improve slightly.
- Certain collaboration with other CoE exists.
- Discussion meetings between the MHCoE and other CoEs seemed to be scheduled for 07.
- The coordination and collaborations with external organizations (even international) is not yet planned as a CoE need, but it is left to the various projects and participating organizations (as in the case of UH through IEA).
- Need more coordination with other groups.
- It was not clear from the presentation if any technology transfer occurs outside the CoE.

Strengths and weaknesses

Strengths
- The CoE is well structured with an excellent integration of expertise and competence to be conveniently integrated on specific topics.
- The coverage of the key most promising materials is guaranteed by the level of competence of the participating organizations.
- The scientific approach is excellent.
- The contribution of the engineering analysis and design adds value and gives substantial tools for material selection towards DOE 2010 objectives.
- Strategy of material research toward the system target.
- The flexible overall structure and the milestone management style enable effective research.
- Good communication and collaboration within the center.
- Team, organization, theory guidance.
- Good approach to project management.
- The CoE is flexible to change as the down-select procedure narrows the group of potential materials.
- Strong group of expert partners with diverse capabilities. Projects are organized, well managed, and have an accurate perspective on the key development areas. Close coordination between theory and experiment has been useful in characterizing existing and guiding new materials research.

Weaknesses
- Unfortunately, project scope is limited by materials (metal hydrides) that have very little potential for large scale commercial on-board applications with the exception of just a few options.
- The CoE does not seem to be well organized, according to the hard-to-follow presentation.
- Lack of clear decision processes and criteria for material selection.
- Risk of overlapping/duplication of theoretical analysis for material investigation, with no clear directions from the Theory Group.
- Lack of a clear and well defined pathway to achieve DOE 2010 targets.
- Down-selection criteria were not well defined.
- Tough problem to solve. Internal communication could improve, for example SRNL science seems almost independent.
- Clear future directions are not completely apparent, however the partners are highly innovative and therefore research is expected to be fairly well-guided. Some additional cross-validation of measurements should be initiated, especially between SNL and the other partners.

Specific recommendations and additions or deletions to the work scope

- Have they considered adding a group to look at binary or ternary systems discussed in other presentations?
- Facilitating go/no-go decisions regarding complex metal hydrides, amides/imides and destabilized hydrides. Perhaps, more effort can be shifted towards AlH_3 (including synthesis, modification and regeneration) and engineering as well as more exploratory work for lead generation.
- Only projects D (AlH_3) and E (Engineering) seem to have enough potential to continue.
- The system-related approach (Project E) must be extended and used as a selection criterion of the investigated materials in any CoE Project.
- The focus on very promising materials requires the definition of clearer plans for material selection or cancellations, in agreement with DOE targets and barriers.
- The various materials with promising performance must have a critical review analysis with relation to the complete set of DOE objectives and technical barriers (not only hydrogen density) to accelerate selection and screening.
- The high theoretical capacity must be better utilized by giving a substantial role to the Theory Group.
- External collaborations in the key research areas of the advanced hydrides investigated must become a central activity of the CoE and not a casual opportunity of single participant contacts.
- Need to leverage the expertise from Sorption Center to develop more innovative ideas.

- A more structured exchange of information and contacts with external potential contributors should be part of the scope of the CoE work to better assist internal R&D.
- The theory predictions need to break down by each step rather than averaging all the steps.
- Incorporate routine theoretical examination of stability and reaction pathway energetics for all compositions to provide experimentalists with best possible material candidates.
- Specific program to refine theory with combinatorial program to test predictions of delta H and decomposition temperature and reversibility.
- Include kinetics component to work portfolio.
- Need to focus on kinetics improvement.
- In the future this talk needs to be more on the management of the center and less on the technology which your PIs will talk to later in depth. Technical accomplishments should be more how the progress relates to goals.

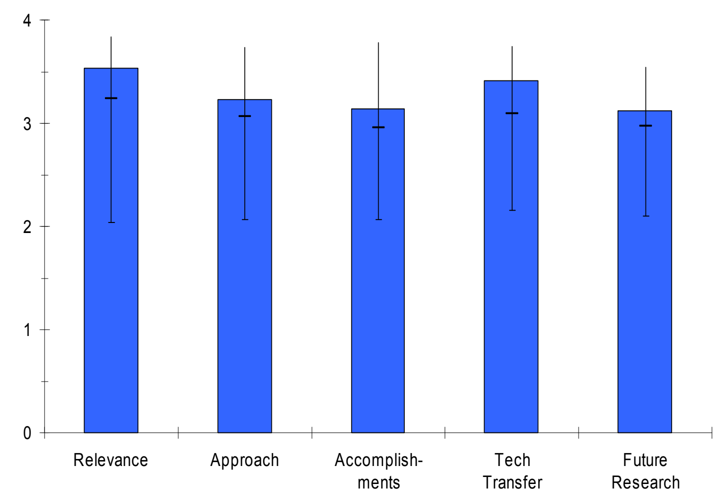
Project # ST-15: Sandia Research as part of the Metal Hydride CoE

Ewa Ronnebro, Eric Majzoub and Tony McDaniel, presenting; Lennie Klebanoff, Mark Allendorf, Jay Keller, Sandia National Laboratory (SNL)-Livermore CA

[NOTE: This review is for Sandia's technical contribution to the MHCoE.]

Brief Summary of Project

Overall Project Score: 3.3 (6 Reviews Received)



Metal hydride research at Sandia National Laboratories continues to develop new high-capacity hydride materials capable of achieving at least 6 wt.% hydrogen for vehicular applications (system basis). Sandia employs a parallel approach through work in each of the following areas: (1) Investigate new complex hydrides and other reversible hydride-based materials to achieve higher capacities; (2) Develop new synthesis and doping processes to improve both absorption/desorption kinetics and ultimate capacity; (3) Experimentally characterize the materials' properties; (4) Determine hydriding mechanisms through experimental analysis and modeling; and (5) Determine important engineering materials properties to ensure that complex hydrides are on track for eventual commercialization.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

- As a member of the MHCoE this project is focused directly on the DOE storage material performance targets.
- This project is apparently playing a key role in MHCoE activities.
- The project is well committed to reach DOE objectives by concentrating on best materials adapted to targets and discovery of new ones.
- The new hydrides can be faster and better screened with the newly developed equipment: this may reduce selection time.
- Identifying new and promising reversible metal hydrides is very relevant to meeting the 2010 targets.
- Materials being studied appear to have potential to meet DOE objectives.
- Relevant work because these are high capacity materials. However the energy required is very high and must be attacked aggressively.
- Project is relevant to DOE objectives.

Question 2: Approach to performing the research and development

This project was rated **3.2** on its approach.

- The approach is well-balanced between theory and experiment.
- The present emphasis on Ca-B-H system at 700 bar after no-go on Na-B-H system demonstrates flexibility and adaptability in the approach.
- The approach is adequate and some suggestions can be referred to the possibility to better focus, immediately after the synthesis and optimization of new materials, to operating conditions (temperature for example) closer to the DOE targets.
- The Monte Carlo method should be compared with the other theoretical methods applied in other projects of the CoE.

- New materials and catalysts are needed and they seek them. This is good. Theory guided experiment is also a good approach to use. Not looking for a CaLiB system is a good example.
- All the "low hanging fruit" aspects of the metal hydride systems have been explored, so the project is seeking to widen the search through a combinatorial approach guided by theory.
- I like the combinatorial approach but would like to have seen more substantial progress on new materials compared to last year.
- Micro-reactor approach has advantages and disadvantages; possible limitations of the approach have not been discussed in detail.
- Stability assessments provide valuable basic information; this work should be continued.
- It is not clear whether the solid-state approach can be scaled up.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.1** based on accomplishments.

- Good progress to date in both theoretical and experimental efforts.
- New high throughput/combinatorial methodology is a strong addition to the experimental effort.
- The progress is well described with a clear vision of the potentialities (closing activities on Na-Si-H is an example of the vision).
- The identification of the reversible calcium borohydride material is interesting, and potentially important if temperatures and regeneration pressures can be reduced.
- Good progress has been made on the combinatorial synthesis system.
- $Ca(BH_4)_2$ system is a good result but needs to be modified to lower temperature and pressure obviously. The Monte Carlo theory work has come along nicely and is contributing in a meaningful way – probably the best result of the period. It is good that the hot plate system is working but it has taken rather a long time to get going. Ge hydride may have a future – it is odd that the TGA is known but the capacity is not.
- $1.8M budget, so should get a fair amount done, score would be higher if this was done on a more modest budget with fewer people.
- Technical accomplishments are at a very high level. However, there are gaps in the understanding of chemical processes taking place during the operation.
- Theoretical assessments require additional experimental support.
- High-throughput screening requires additional validation.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.4** for technology transfer and collaboration.

- In association with the Metal Hydride Center, the project has many important collaborations in place.
- Significant collaborations both within and without the CoE.
- A patent application has been filed.
- The focus is mostly on research activities with adequate collaboration described with research organizations.
- There is no clear description of possible industry involvement, due to the early stage of development and IPR concern.
- Highly connected with team members of the center, but also with outside groups. Could improve by using those connections more frequently and directly to get results.
- Collaboration with academic institutions is very good. However, there is plenty of room for the collaboration with industry.
- Technology transfer is good within SNL but it was not clear from this presentation if any technology transfer is occurring outside SNL.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.1** for proposed future work.

- Future plans thoroughly developed and appropriate.
- The future plans are clear and well organized.
- There are a few doubts about the way some technical limitations of present materials will be solved or addressed (as, for example, in the case of amides).
- If the December 2007 decision is a no-go on the complex hydrides currently under study, then the project is essentially back in search mode for complex hydride materials that have a possibility of meeting the 2010 targets.
- Will there be enough information known about significantly reducing the temperature and pressure of the calcium borohydride by the materials down-select date?
- The combinatorial system for elevated temperature synthesis uses a silicon container. Are reactions with silicon a limiting factor for exploring some systems?
- The ability to drop unfruitful research is laudable and shows planning and the ability to follow them. Theory guide to research is a good move. Plans are clear and appropriate with the exception of what I think is insufficient emphasis on catalysts.
- Future work is formulated in very general terms. It is not quite clear which materials are going to be studied in detail.
- Nano-engineering: no explanation is provided; it is not quite clear how the group is going to design novel nano-materials.

Strengths and weaknesses

Strengths
- Strong team with demonstrated expertise in their respective areas of responsibility.
- The project is well organized and directed with a well-justified approach and with high level of competence and skills.
- The resources are adequate with a very good complementarity.
- Well planned and coordinated project.
- Materials that have little chance of working are quickly discontinued.
- Combinatorial synthesis technique should lead to rapid screening of potential candidates.
- Calcium borohydride is a promising material if rehydriding step can occur at less severe pressures.
- Theory is making good progress and they are developing new materials. They have repeatedly shown they can cut off lines of work that are complete or unproductive. High capacity of targets is suitable. Use of theory to scan formulations and enhance “hit rate" is very good, keep the computer busy!
- Team communicating and functioning better than last year, they are back on track and that is good to see.
- Collaboration with research organizations is quite impressive.
- Theory-experiment relationship.
- High-throughput screening approach may become extremely useful.

Weaknesses
- Does theory lead or follow the experimental work? To date it appears the focus has been to use experimental data to validate the theoretical model-hopefully in the future the theory work will be used to guide and direct the experimental effort.
- Project seems to be a little short on creative ideas.
- Energy and temperature “sum it up”. Delta H “kills” systems at release temperatures above 100°C because all the energy must come from stored hydrogen as the team is well aware. They need to find lower enthalpy and temperature materials to succeed. Combinatorial system was rather slow in coming on line.
- Marginal collaboration with industry.
- Understanding of chemistry involved in the operation of B-based materials has room for improvement.

Specific recommendations and additions or deletions to the work scope

- I presume that work involving calcium borohydride rehydriding has occurred with high purity hydrogen. They could consider looking at less pure hydrogen systems to see if there are inhibitors or synergies in the rehydriding step.

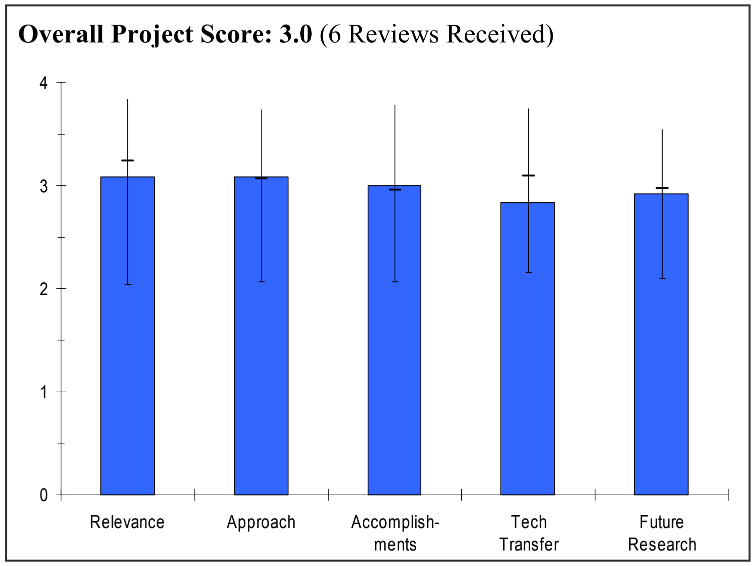
- The preparation of $Ca(BH_4)_2$ in the solution should be explored in more detail.
- Since diborane is usually accompanying transformations of borohydrides, its formation during the operation of potential candidates should be evaluated in very early stages of the research.
- Need to approach catalysis more formally. So far the so-called mixed or destabilized hydrides have not lived up to their thermodynamic possibilities in part because the kinetics behave as if the energy barrier is unaltered, and this is not so unlikely as the thermodynamic advantage comes on the products end of the reaction – transition states may be only weakly influenced by the modifications. Use hot plate to look at catalysts rapidly.
- None.

Project # ST-16: Lightweight Intermetallics for Hydrogen Storage
J. C. Zhao; General Electric

[Member of the Metal Hydride Center of Excellence]

Brief Summary of Project

The objective of this project is to discover and develop a high capacity (> 6 wt.%) lightweight hydride capable of meeting or exceeding the 2010 DOE/FreedomCAR targets. Specific objectives for fiscal year 2007 include performing combinatorial and computational screening of catalysts, dopants and complexes for $Mg(BH_4)_2$, and exploring ways to make the materials reversible.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.1** for its relevance to DOE objectives.

- This project clearly conforms to the President's Hydrogen Fuel Initiative and DOE's Multi-Year RD&D plan by seeking a new and cheap high-capacity storage material with low-temperature H_2 recovery and critical reversibility.
- High wt.% push stated, but little said on volumetric and other properties.
- Work is relevant to DOE goals for gravimetric and desorption goals but it is not clear what has been accomplished for volumetric and refueling goal.
- I assume that cycle life would be affected by by-products, but it was not clear from the presentation if this is being considered.
- High capacity materials that are not made from expensive precursors are good. Need to seek lower delta H while also seeking reversibility - not an easy task.
- Project is relevant to DOE objectives.

Question 2: Approach to performing the research and development

This project was rated **3.1** on its approach.

- The project has progressed to the point of down-selecting to three materials that can meet weight targets: $Mg(BH_4)_2(NH_3)_2$, $Mg(BH_4)(AlH_4)$ and $Mg(BH_4)_2$. These are basically different from materials in most other DOE programs.
- This is an acceptable high-risk approach. All of these materials have significant problems to overcome, not the least of which is reversibility. Project is focused, for sure.
- High-throughput screening is useful.
- Efforts spent on catalyzing $Mg(BH_4)_2$ are not clear. Thermodynamics limitations of the borohydride stability have to be addressed first.
- Reasons for using borohydride based catalyst, synthesis routes for $Ti(BH_4)_3$ and its stability are a concern!
- Theory base is not made clear. Seems more or less like mixing the usual suspects - not all bad, but not highly enlightened either. High throughput work is a good way to improve progress.
- Too strong emphasis on a Mg-B-H system.
- New ideas are highly desirable.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- Significant progress has been made in understanding the three down-selected materials relative to the technical barriers.
- Catalysis has shown some beneficial effect, but $\Delta T = -50^{\circ}C$ seems disappointing.
- Most RGA outgassing results show traces of boranes and $Mg(BH_4)_2(NH_3)_2$ shows significant NH_3 (and related NH_2). Does this mean that supplementary H_2 purification will be required at an increase of system weight?
- Finding new materials through the high-throughput method is very smart.
- Energy to generate hydrogen seems too high, need to find either a low temperature or low energy material.
- It would be good to see more work on the reformation reactions.
- I would like to see catalysis work to smooth out the $Mg(BH_4)(AlH_4)$ desorption curve.
- The catalysts did not lower the desorption temperature very much for $Mg(BH_4)_2(NH_3)_2$, so more work here would be useful.
- Assumptions of compound formation need to be differentiated from confirmed formation of compounds or structures, i.e. $Mg(BH_4)AlH_4$ type of compound is just an assumption and this need to be more clear in the presentation.
- Catalyst studies purposed for both $Mg(BH_4)_2(NH_3)_2$ and $Mg(BH_4)_2$ when the main problem is of a thermodynamic nature, the reason is not clear.
- Getting some reversal in the system is good and the materials being tried are not unreasonable. Appropriate to look for catalysts, no huge change in hydrogenation but a needed search. Structure determination seems to be more of basic science interest, not of much practical interest. Still need to find a reversible system – did improve some in this regard.
- NH_3 and AlH_4 incorporation was worth a try. Did improve the release temperature this way.
- An excellent work on the preparation and characterization of $Mg(BH_4)_2$.
- High-throughput screening is not discussed in sufficient detail.
- Scalability of $Mg(BH_4)_2$ synthesis has not been discussed. Is the synthesis scalable?
- $Mg(BH_4)(AlH_4)$ is not sufficiently characterized.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.8** for technology transfer and collaboration.

- Good collaborations shown nicely in slide 2 and the various results slides.
- Useful position, at least on paper, in the MHCoE.
- Given the fact BNL (Brookhaven NL) is listed as the source of data on several results slides, why is it not listed as a formal collaborator in slide 2?
- Since this project is in an early phase, technology transfer to other groups is likely not appropriate at this time.
- Collaboration with other members synthesizing borohydrides, amides and alanates systems is not so visible.
- Seems well connected but a more "cards close to the vest" program than most in the center, possibly because of corporate IP concerns. Could be improved, but not likely to occur.
- Collaboration with other research institutions is at much higher level than that with materials manufacturing industry.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.9** for proposed future work.

- In spite of high risk, no changes suggested in work plan for future.
- Plans clearly based on past results and are sharply focused on technical barriers.
- Reviewer appreciates the built-in go/no-go decision points. It would be even better if they could be made more quantitative.
- Guidance of future materials research is not clear

- It would be useful to see goals and plans for reformation work since it was stated that no catalyst has been found to enable the $Mg(BH_4)_2$ reaction and $Mg(BH_4)_2(NH_3)_2$ is only partially reversible.
- Fairly suitable as far as it was detailed, but not fully clear exactly what will be done from the plan listed. Should try to decrease delta H.
- Future work is formulated in very general terms.
- It is not quite clear why work on Mg-B-H system should continue. Experimental results presented suggest the opposite.
- New ideas could significantly benefit this project.

Strengths and weaknesses

Strengths
- Looks at high-capacity borohydrides capable of meeting system weight targets.
- Good researchers and collaborations.
- Efficient combinatorial experimental approach.
- High throughput equipment seems to speed up the searching process but need idea.
- Good program for looking at desorption.
- Good system to focus on based on capacity.
- Collaboration.
- Very solid experimental work.

Weaknesses
- The borohydrides are a difficult and high-risk approach, with many problems to be solved, including high desorption temperatures, poor reversibilities and impurities in the H_2 released.
- This reviewer would have liked to see more information on volumetric H-densities.
- Need more work on material reformation.
- Addressing the real problems related to the materials researched.
- May never get full value due to isolation they seem to need for internal reasons. Energy requirements are a big problem in these systems and catalysts are sorely needed.
- Focus on only one group of materials.
- Since diborane is usually accompanying transformations of borohydrides, possibility/extent of its formation during the operation of potential candidates should be evaluated in very early stages of the research.
- Marginal collaboration with materials manufacturing industry.

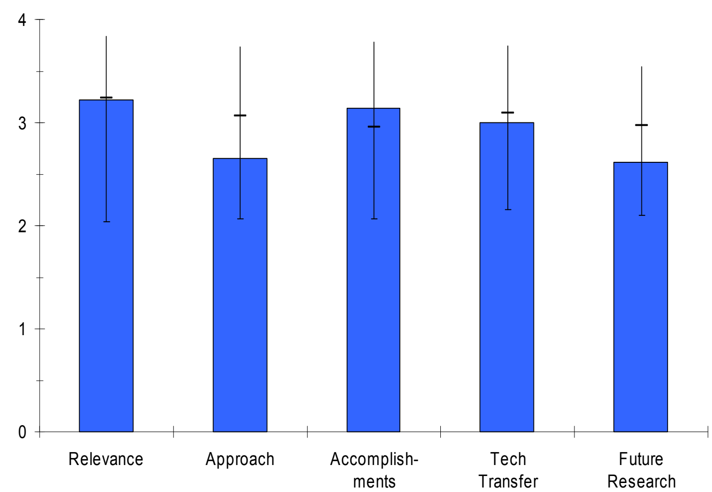
Specific recommendations and additions or deletions to the work scope

- Why not consider partially substituted $Mg(BH_4)_2$ rather than catalyzed $Mg(BH_4)_2$?
- With significant ammonia formation, why continue with $Mg(BH_4)_2(NH_3)_2$?
- Recommend to confirm formation of $Mg(BH_4)(AlH_4)$ prior to any catalyzation trials.
- Recommend to collaborate more with other members of the center.
- Focus more on catalysts and getting reversibility. Also need to focus on lower delta H. Theory guide may help here. Consider carefully what the criteria are for getting out of the Mg-B area. Leave off some of the interesting but un-used testing such as structural determinations.
- go/no-go decision about $Mg(BH_4)_2$ should be met as soon as possible; preferably by July-August 2007.
- No change.

Project # ST-17: First-Principles Modeling of Hydrogen Storage in Metal Hydride Systems
Karl Johnson; Univ. of Pittsburgh, David Sholl, Co-PI, Carnegie Mellon University

[Member of the Metal Hydride Center of Excellence]

Overall Project Score: 3.0 (6 Reviews Received)



<u>**Brief Summary of Project**</u>

The objectives of this project are to 1) compute thermodynamics of metal hydride systems, 2) compute interfacial properties of hydrides, and 3) address fundamental processes in hydrogenation. Specific objectives for fiscal year 06/07 include:
• Identify promising complex hydride materials through computational screening of the heat of reaction ΔH;
• Develop an automated approach for identifying all possible compounds from a given set of reactants and products;
• Screen doped hydrides for phase stability;
• Initiate calculations for ΔH of substituted (doped) complex hydrides, including $Mg(BH_4)_2$and $Ca(BH_4)_2$;
• Compute surface reactions as relating to poisoning and initial kinetics of hydrogenation/dehydrogenation;
• Contribute to the development of CALPHAD databases for metal hydrides.

<u>**Question 1: Relevance to overall DOE objectives**</u>

This project earned a score of **3.2** for its relevance to DOE objectives.

- In the metal hydride field, one thing that is needed is high capacity reactions with suitable thermodynamics for efficient thermal management considerations. This work is directed at this goal.
- The project involves computational studies of metal hydride system thermodynamics, interfacial properties that relate to adsorption/desorption of hydrogen, and energetics of hydrogenation. This type of information has great value in the context of what the CoE for Metal Hydrides is trying to accomplish.
- The project provides valuable screening capability that can sort through large numbers of chemical phases in search of the most promising candidates for hydrogen storage.
- A variety of issues related to hydrogen storage that require information on molecular energetics are under study.

<u>**Question 2: Approach to performing the research and development**</u>

This project was rated **2.7** on its approach.

- Predictive modeling approach is a promising, cost-effective way to accelerate discovery of novel storage reactions.
- Modeling needs to address not only candidate hydride materials, but a systematic predictive method for identifying the lowest-energy thermodynamic pathways. This latter approach is missing in the current project, and has led the PIs to predict spurious reactions.
- It is not clear on what basis the selection criteria were chosen. Based on previous DOE presentations, it is recommended to narrow down the selection to 0-100C equilibrium temperature and 15-30 kJ/mol H_2 enthalpy.
- >160 solid materials, ~350 reactions … This is not an efficient approach. On the other hand the theoretical methodology is the state of the art.
- State-of the-art DFT packages are used to perform calculations of free energies and other thermodynamic quantities for a wide variety of chemical compounds and molecular architectures.

- Wherever possible, the computational results should be compared with existing experimental data. Agreement with experiment adds credibility to all aspects of the work.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.1** based on accomplishments.

- The prediction of novel high-capacity reactions is quite important and will help direct experimental efforts towards promising materials. However, the PIs appear to be using mainly chemical intuition to describe the lowest-energy decomposition pathways. This intuitive approach has led in several cases to predicted reactions as being "single step" reactions with suitable thermodynamics, when in fact they are thermodynamically "multi-step" reactions, each of which has unsuitable thermodynamics.
- A lot of work has been done. The database will be useful.
- Kinetics of multiphase reaction systems is expected to be controlled by solid-phase diffusion as well as surface reaction. They should consider easiness of solid-phase diffusion in the system studied.
- The poisoning studies of complex metal hydrides are very useful.
- Thermodynamic quantities are computed with reasonable accuracy.
- Several potentially interesting reactions have been identified.
- A broadly useful data base is evolving from this work.
- The interfacial energy calculations are particularly worthwhile for sorting out hydrogen uptake and release issues.
- It's no big surprise to find out that elements that “like” hydrogen also “like” oxygen.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- It was not clear who is the end-user of this work and how the data impacts their work.
- Can the PI provide specific examples on how this work helped the synthesis/experimentalists in the center?
- A stronger collaboration with experiment will help in strategy.
- Collaboration apparent with HRL, University of Utah, GE and SNL.
- There was some mention that experimentalists in the Metal Hydride CoE are following up on the findings from this project. That's what should be happening.
- The level of collaboration should be broader than is obvious from the presentation. For a project like this, i.e., one that provides both screening results and energy parameters, there should be cross-collaboration in virtually all task areas.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.6** for proposed future work.

- Future work seems to be largely comprised of "concluding" or "completing" various tasks, rather than novel, creative approaches.
- The development of an automated approach will not solve the hydrogen storage problem!
- The database will be generally useful.
- They should include an activity to investigate the effect of solid-phase diffusion in their system.
- The proposed future work on Slide 21 is presented in a very general way. Try to be more specific in the future. What will be done? Why? Which other CoE projects will it contribute to?
- The doping studies and the interfacial studies should be emphasized.
- Any calculations you can do that relate to or give information about kinetics will have great value.

Strengths and weaknesses

Strengths
- Computational capabilities.
- The PI is very knowledgeable.
- The publication record is impressive—particularly the Science article. That's a "kudo" for the CoE.
- Much is learned per-dollar of funding in projects like this one.

Weaknesses
- Methodology.
- Information exchange on reaction in solid phase between the theoretical side and the experimental side seems not to be so effective.
- There are no obvious weaknesses in this project, but a more explicit demonstration of the interplay with the rest of the CoE would raise the project's visibility level.

Specific recommendations and additions or deletions to the work scope

- A more strategic and efficient approach is needed.
- Support understanding and directing experimental results with aid of calculations is definitely recommended to continue.
- See the recommendations given in the comment boxes above.
- Modeling needs to address not only candidate hydride materials, but a systematic predictive method for identifying the lowest-energy thermodynamic pathways. This latter approach is missing in the current project, and has led the PIs to predict spurious reactions.
- Need to further validate the model with established samples within the above range. (0-100°C equilibrium temperature and 15-30 kJ/mol H_2 enthalpy).
- In next year's presentation, provide indications of how each computational task relates directly to ongoing experimental work within the CoE or is connected to an issue of importance to other CoE projects.

Project # ST-18: Thermodynamically Tuned Nanophase Materials for Reversible Hydrogen Storage

John Vajo, presenting; Ping Liu (PI); HRL Laboratories

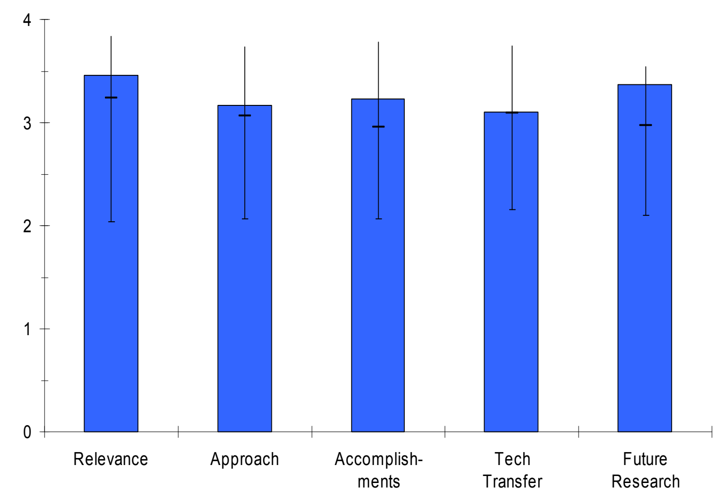
[Member of the Metal Hydride Center of Excellence]

Brief Summary of Project

The overall objective of this project is to develop and demonstrate a safe and cost-effective light-metal hydride material system that meets or exceeds the DOE goals for reversible on-board hydrogen storage. Specific objectives for FY2006/2007 include:

- To identify and test new high capacity Li- and Mg-based destabilized hydrides;
  - o Screen candidate $LiBH_4$ + MgX destabilized systems and evaluate energetics and kinetics,
  - o Down-select systems for additional work;
- To apply nano-engineering methods to address kinetics limitations;
  - o Determine hydrogen exchange rates in nanoscale MgH_2/Si,
  - o Evaluate sorption kinetics and thermodynamics of $LiBH_4$ and Mg in carbon aerogel scaffolds,
  - o Assess capacity penalty for hydrides in scaffolds (can they be practical?).

Overall Project Score: 3.3 (6 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

- The objectives are relevant to DOE's overall objectives in pursuing the Hydrogen Fuel Initiative.
- The project is well in line with DOE objectives.
- The conclusion of the project at 2010 makes slightly unclear possible references to 2015 targets (in extra slides).
- Project conforms very well to President's HFI and DOE Multi-Year RD&D plan.
- Project aims at meeting targets for weight, volume and H_2 delivery temperatures, as well as cost and safety.
- The $LiBH_4$ - MgH_2 system may have a possibility of meeting the 2010 targets.
- The project, aiming to develop a high-capacity storage material working at ambient temperature, fits well to the DOE objective.
- Highly relevant work, one of the key thrusts in the center now.

Question 2: Approach to performing the research and development

This project was rated **3.2** on its approach.

- The project is a difficult one. It may have high payoff.
- The PI needs to focus on 1) Mg-in eutectic 2) catalysts 3) effect of high pressure on aerogel.
- The approach is acceptable with clear steps to improve key performance and limitations.
- The emphasis on cost and safety is not yet considered.
- Effort is focused on two most important technical barriers associated with light metal hydrides - thermodynamics and kinetics.
- Thermodynamics controlled by "destabilization", the mixing of secondary reactants (e.g., MgH_2 to $LiBH_4$) to provide an exothermic contribution to the otherwise highly endothermic desorption.
- Kinetics controlled by nano-sized particles.

- Carbon scaffolds applied to maintain small particle sizes.
- Very good combination of approaches to attack barriers.
- Scaffold approach is a good one to attempt to maximize the kinetics of the $LiBH_4$-MgH_2 system.
- Approach based on their own concept of 'destabilization' is successful for exploring reactions with small reaction enthalpy.
- Poor kinetics is the most serious problem. Nano-engineering that they started is expected to provide some knowledge about the effect of particle size and diffusion distances.
- Solid approach, might benefit from greater guidance from the theory team in the center. For some reason the thermodynamics used are not working as expected and perhaps a different level of theory [guide] would help.
- Scaffold use is another center showpiece that came from this group.
- Willing to make or accept a no-go on their own work.
- Some indication that there is a thermodynamic improvement too, likely due to chemical interaction.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.2** based on accomplishments.

- This project is an excellent example of following the work plan, objectively reporting both negative and positive results, and eliminating R&D directions that are clearly not promising.
- Since it is a difficult project, a lot of work is needed to show progress. Using nanophase brings up the issue of safety, which was not addressed.
- The results and the progress are interesting.
- The operating conditions (e.g., 300°C) are not compatible with the DOE targets.
- Project has accomplished much of what was planned, with both positive and negative results.
- $LiBH_4$ + MgX combinations, so far, not very useful for destabilization.
- No-go decision made on MgH_2 + Si system. Attempts to utilize several approaches failed to achieve reversibility.
- Preliminary results to test C-aerogels as scaffolds are very promising relative to decreasing desorption temperatures and increasing kinetics (better thermodynamics?). Cyclic capacity loss still a problem, as well as carbon scaffold penalties.
- No new destabilized $LiBH_4$ systems have been identified, other than the MgH_2 destabilization.
- Looks like it is difficult to get Mg into the carbon aerogel, but multiple approaches are being pursued to address this.
- Possible evidence for aerogel scaffold effects on the thermodynamics of $LiBH_4$.
- The result of exploring new combination for 'destabilized' reaction is rather poor.
- The trial using carbon aerogel as scaffold shows good indications for desorption pressure and kinetics.
- Scaffold work to reduce [attach] temperature of dehydrogenation is very good. Pore size work is likely giving clues as to the optimal function of the aerogel, for this application and perhaps generally. Getting Mg in carbon aerogel is a difficult thing to do and they appear to have done it, results will be interesting.
- Also did work on MgSi and 2 other systems that did not produce a winning compound but were reasonable systems to try based on theory.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.1** for technology transfer and collaboration.

- The coordination and roles of participating organizations is very good and adequate to the needs.
- Good collaborations within MHCoE and outside.
- Very good collaboration with regard to carbon aerogels.
- Collaboration with the groups synthesizing scaffolds works well.
- Well connected internally and externally.
- Positive results with LLNL aerogels cited, but LLNL is not listed as a formal collaborator in Slide 2.
- PI needs better collaboration with partners.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.4** for proposed future work.

- Looks good.
- The future plans are well consistent with the current limitations.
- Plan builds nicely on past results and stays completely focused on technical barriers.
- PI's Program Direction matrix slide (16) is an excellent display of past, present and future.
- Future work with the carbon aerogels is well-structured.
- What is the "Plan B" if the carbon aerogel approach does not work out?
- Approach using scaffold materials should be more focused and done more systematically.
- How to explore the combination of materials for 'destabilization' is not necessarily clear.
- More attention to DOE targets is required.
- Appropriate. Working on thermo, kinetics and capacity.

Strengths and weaknesses

Strengths
- The project has good potential.
- Clear vision of the current material limitations with reasonable research plans.
- Destabilization and the concurrent use of nanoporous scaffolds represent an important approach to attack the thermodynamic and kinetic barriers. In spite of inherent metallurgical problems (see below), the project must be completed as planned.
- Project participants are very competent and unusually skillful at designing and executing a multifaceted R&D approach.
- The $LiBH_4$-MgH_2 system has the potential to meet the 2010 targets, if the kinetics can be significantly improved.
- The PI has started to prove their original idea of 'destabilization'.
- Great ideas and strong team

Weaknesses
- The proposed research lines do not guarantee the reach of the targets.
- The only project weakness is nature itself. It will be very difficult to get good room-temperature reaction kinetics when the diffusion of metal species is involved. Nano can only go so far.
- There may be no other destabilizers for $LiBH_4$ other than MgH_2.
- Approach for improving kinetics is limited.
- Needs a lot of work.

Specific recommendations and additions or deletions to the work scope

- Maybe testing more chemical systems in the scaffold would be good.
- Introduction of supporting cost and system analysis as a mandatory task of a member of the MHCoE.
- No changes recommended.
- None.
- Exploring of 'destabilized' reactions should be tailored to some new kinds of materials.
- Get the theory team at the center to try to refine the destabilization predictions so as to make it a more accurate guide.

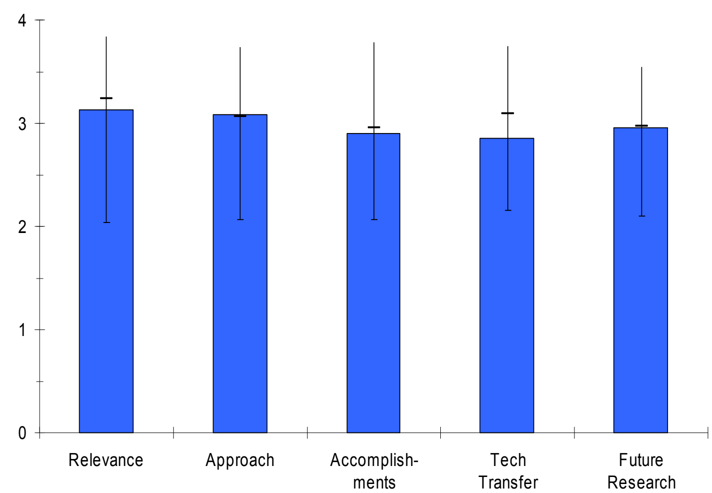
Project # ST-20: Synthesis and Characterization of Alanes for Automotive Applications

Jason Graetz (PI), presenting; Jim Wegrzyn (co-PI), J. Reilly, J. Johnson, W. Zhou, Brookhaven National Laboratory (BNL)

[Member of the Metal Hydride Center of Excellence]

Brief Summary of Project

Overall Project Score: 3.0 (6 Reviews Received)



The objective of this project is to understand the strengths/weaknesses of using aluminum hydride (AlH_3) as a storage medium by quantifying the reaction kinetics, thermodynamics, and energy requirements for regeneration. This will be done by synthesizing 3 polymorphs of AlH_3 (α, β and γ) with material capacities $\geq$ 8% kg-H_2/kg (grav.) and $\geq$ 0.10 kg- H_2/L (vol.). AlH_3 polymorphs with suitable H_2 pressures at temperatures near the operating temperature of a proton exchange membrane (PEM) fuel cell (~85°C) will be identified and it will be determined if AlH_3 can be formed by direct high-pressure hydrogenation of Al powder at pressures <103 bar. Specific objectives in fiscal year 2007 include:

1. Produce aluminum hydride with 9 wt. % H_2 and 0.13 kg H_2/L (material capacity);
2. Develop practical and economical process for the regeneration of AlH_3 from the decomposed Al;
3. Assist in the design for an on-board fuel tank delivery system.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.1** for its relevance to DOE objectives.

- High capacity and low enthalpy of dehydrogenation make alane a viable option to investigate for on board storage.
- The objectives are relevant to DOE's overall objectives in pursuing the Hydrogen Fuel Initiative.
- In line with RD&D program objectives and addresses a number of key barriers.
- Very relevant. Addresses one of the main barriers to commercialization of H_2 vehicles.
- The high capacity meets the DOE target. Studying possibility of using this material is relevant to the total program.
- Good program direction; well aligned to goals. A good material to study.

Question 2: Approach to performing the research and development

This project was rated **3.1** on its approach.

- Excellent idea of using organic adducts to lower the pressure for hydrogenating Al.
- Perhaps needs more systematic approach for developing most optimal organic adducts that would be easier to remove from AlH_3 without loss of hydrogen (modeling?).
- The project is well designed. AlH_3 has potential, but regeneration is a big problem.
- Addressing the problem via liquid organometallic is good.
- Reasonable and well-thought-out approach focused on regeneration and possible routes.
- Regeneration energy requirements established for the screening on possible pathways.

- Addresses a key issue for alane system-regeneration.
- Have identified a regeneration approach that is promising.
- Focused approach-have eliminated work on LiCl splitting due to energy requirements that are too high.
- Characterization of the material is essential to know possibility of its use.
- Rehydrogenation is a real key issue and needs to be focused on.
- Seem to understand the key questions and are focused on improving those aspects (temperature and reversal in particular). Regeneration target energy is a bit higher than I would like to see. For example, it is higher than gas compression and slightly higher than liquefaction.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.9** based on accomplishments.

- Project seems to be on track, however at this early stage it is difficult to predict if most important targets could be met with the approach.
- Good.
- Good progress in understanding the regeneration process and properties of AlH_3 for H_2 storage.
- Significant accomplishment with the direct hydrogenation of activated Al powder with a ten-fold reduction in pressure and a yield of almost 100%.
- Have reduced hydrogenation pressure and temperature by using tetraethylenediamine complex (TEDA), but have not demonstrated decomposition of TEDA adduct to give back AlH_3.
- Structural/thermodynamic studies provide needed information.
- Progress toward a useful reversible system is slow.
- Characterization has been almost accomplished except for detailed investigation how kinetics is controlled by the surface condition.
- The trial of regeneration in organic route has a lot of problems to be solved.
- Some progress on recycle, making AlH_3*TEDA. Did finish phase study. Progress might have been greater based on funding level.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.9** for technology transfer and collaboration.

- Strong collaborations within the Sorption CoE, the Chemical Hydride CoE but also at international level.
- Thanks to its networking this project profits from wide-range, top-class expertise and access to unique material characterization facilities.
- Collaborations evident in structural studies.
- Additional collaboration with theory group and chemical hydrogen storage center would be beneficial.
- International collaboration present.
- No results from collaborations with SRNL and UH on regeneration yet.
- PI needs more collaboration with partners.
- Collaboration works well on both characterization and exploring various way of regeneration.
- Good outside and inside connections, probably better outside actually.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- Looks good.
- The path forward is planned in a sensible manner based on findings to date and capitalizing on the expertise of collaborators.
- Clear milestones and go/no-go decision points have been set.
- Collaboration with Chemical Hydrogen storage center should be beneficial.
- Not sure what additional fundamental high-pressure studies are planned and what benefits they will provide – a better description of planned high pressure work would be helpful.

- Pursuit of alane adducts may be beneficial, but it will be difficult to find an adduct with the high hydrogen storage density needed. Must be careful in adduct choice so that elimination reactions upon adduct decomposition do not occur (would lead to impurities in H_2 and Al-products that would be more difficult to convert back to AlH_3, and would probably need off-board regeneration).
- Focusing on rehydrogenation is reasonable. Trying to find a complex containing AlH_3 is one approach.
- The proposed 'reversible metal-organic hydride' seems difficult to achieve the target of gravimetric capacity.
- Appropriate, though not clear that it comprises $0.9 million in work.

Strengths and weaknesses

Strengths
- Seems to be most relevant approach within Metal Hydride CoE.
- PI has good group.
- Networking and pooling of expertise, technical resources, unique facilities and instrumentation.
- Have made some progress in regeneration, decreasing H_2 pressure needed to a relatively low 35 bar.
- Strong activity and experience for characterization of materials.
- Excellent material and talented team.

Weaknesses
- Lack of strategies for removing TEDA from the AlH_3 other than simple evacuation that would result in losing hydrogen. Perhaps needs some more effort towards understanding of the potential of chemical removal of TEDA.
- AlH_3 has been studied extensively with not much hope.
- Recycling - adapt synthesis route to reuse/reduce byproducts.
- Challenge of tuning the decomposition kinetics.
- It is open question if off-board regeneration of solid hydrides is realistic.
- Cost effectiveness.
- Regeneration is a challenging issue. Solid-gas reaction is most preferable, but energy consuming in pressurized gas.
- Equilibrium T-P curve shows P_{eq} is around 50 bar at 77K. This means AlH_3 system has a larger capacity than the best sorbent materials found so far when using at 77K.

Specific recommendations and additions or deletions to the work scope

- Perhaps need more focus on the use of alane in addition to regeneration/synthesis. Alane is thermodynamically metastable at 25°C below 7 kbar pressure, and may create substantial safety issues for users.
- Since AlH_3 is thermodynamically metastable system at ambient temperature, it would be worthwhile to check the potential for run-away pressure build-up at operating conditions.
- More modeling to define optimum alane-base adduct bond energy to drive hydrogenation but allow recovery of pure AlH_3 would be helpful.
- Feedback from the AlH_3 Theory Group is required - to calculate gas-phase complex stabilities to guide BNL regeneration efforts.
- Explore other activation processes (and use of catalysts) for the Al powder.
- Associated regeneration costs could also be addressed.
- Increase interactions with the chemical hydrogen storage center on regeneration issues and potential hybrid schemes.
- Increase interaction with the theory group.
- The low desorption rate at 80°C is another problem. Kinetics depends on the surface conditions. More detailed investigation of the surface effects on the kinetics is needed. It should be noted that the surface condition would depend on the hydrogenation (regeneration) process.
- A little more planning on what would be the theoretically optimal or better than current ligands would be a wise move, get help from center partners if need be. Still would like a higher efficiency target, in concert with DOE goals.

Project # ST-21: Chemical Vapor Synthesis of Nanocrystalline Binary and Complex Metal Hydrides for Hydrogen Storage – Understanding and Discovery of H_2 Storage Materials Involving Metal Amides

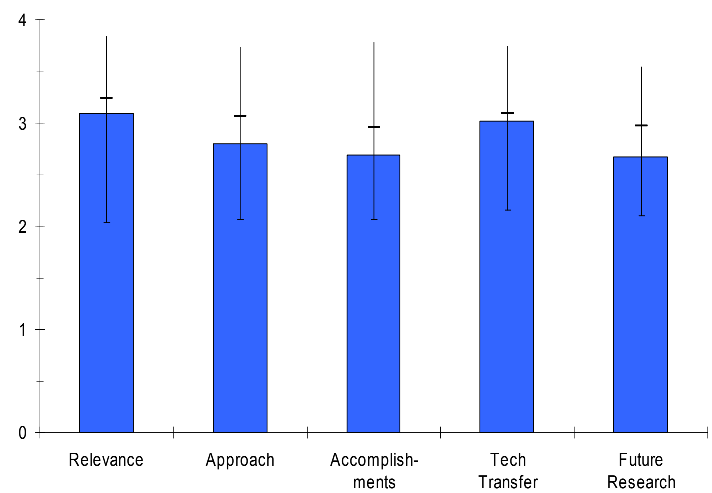
Zak Fang; University of Utah

[Member of the Metal Hydride Center of Excellence]

Brief Summary of Project

The objectives of this project are to discover new solid hydrides that meet reversibility and kinetics requirements, to develop a chemical vapor reaction process (CVS) for synthesis of nano-sized solid metal hydrides, and to demonstrate the effectiveness and unique properties of nano-sized solid hydride materials for hydrogen storage. Specific objectives for FY 06/07 include: 1) discover and study new materials based on lithium alanates destabilized by light metal amides, 2) synthesize new materials using high-energy high-pressure reactive milling process, and 3) synthesize nano precursor and hydride powders using Chemical Vapor Synthesis (CVS) process.

Overall Project Score: 2.8 (6 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.1** for its relevance to DOE objectives.

- The basis of this project is relevant to the scope of the DOE objectives in that it involves both explorations of novel complex hydride combinations as well as new routes for generation of nanocrystalline materials.
- The objectives are relevant to DOE's overall objectives in pursuing the Hydrogen Fuel Initiative.
- Aimed at addressing a number of key objectives from the DOE plan.
- This work is directed at an important goal of reversible metal hydrides: discovery of novel combinations of hydride materials that will produce high-capacity reversible reactions with low enthalpies of decomposition.
- Project is consistent with President's HFI and DOE's Multi-Year RD&D plan.
- Focus on kinetics, H-content and synthesis is good.
- Could perhaps have additional focus on volumetric H-content and processing cost.

Question 2: Approach to performing the research and development

This project was rated **2.8** on its approach.

- While the approach to chemical vapor synthesis (CVS) is novel and has been experimentally proven, the approach toward selection of the two-component complex hydride systems is unclear. On what basis were these compositions chosen?
- Their approach toward characterization and property evaluation for storage compositions involves access to a variety of different (and valuable) techniques (through center collaborations). Nevertheless, given this access, it is not evident that all pieces of data are being interpreted properly or used collectively to clearly deduce reaction mechanisms.
- The project addressed technical barriers such as inadequate kinetic properties and lack of robust synthesis methods, but left out the contamination due to milling process. Previous year suggestion to move away from alanate / amide systems was good, and was not incorporated.

- The PIs appear to have had a few clever ideas of combining two existing ideas in the literature: decomposition of Li_3AlH_6, and the combination of LiH with metal amide materials ($LiNH_2$ and $Mg(NH_2)_2$). The results look quite interesting, though it is not clear how the combination of these two materials will really give results significantly better than the materials separately.
- Very good to see experimental groups quickly synthesizing and testing predictions from the theoretical efforts of the center.
- Although not completely clear in Slide 2 (Barriers), work is properly aimed at important weight and desorption temperature problems with metal hydrides.
- Sensible, targeted approach for exploring the metal amides as hydrogen storage systems.
- The main direction of the project is looking at mixtures of alanates (particularly Li_3AlH_6) and amides (particularly $LiNH_2$ and $Mg[NH_2]_2$). It seems like the limited potential and NH_3 problems of these systems mitigate against full success in metering system targets.
- Work on new materials (e.g. LiMgN) is good, with hopefully lower NH_3.
- The vapor phase synthesis work, particularly in support of the MHCoE seems useful.
- Barriers to utilization of amide systems are not well tackled. Analysis of gases evolved from destabilized/amide based systems should be incorporated in the initial testing steps.
- Purpose for utilization of known synthetic methodology which utilizes high energy high pressure synthesis need to be clarified more, i.e. plan to regenerate AlH_3!

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.7** based on accomplishments.

- In regards to the amide-alanate work, the progress and technical conclusions are lacking. It was not clear what new knowledge has been gained for the $Li_3A_lH_6$-$LiNH_2$ system as compared with FY06. Additionally, a variety of their accessible techniques (i.e. IR and PCT data) did not seem to be included, yet could aid in clearly determining the reaction mechanisms for these amide-alanate systems. There were also several inconsistencies between data and proposed mechanisms (e.g. plateau pressures and extracted delta H's inconsistent with proposed reactions and observed reaction species that were not in mechanisms).
- It was good to see consideration of durability for the materials as exemplified by cycling study.
- The CVS synthesis project seems to greatly support the efforts of the entire center through preparation of precursors. It would be helpful to know the scale and purity of this method.
- The negative accomplishments mentioned, such as limited reversibility of lithium alanate and problems using amide alone are well documented. Using combination of alanate & amide will create problem of NH_3 and should be addressed.
- Significant progress has been accomplished in line with the project objectives.
- Demonstrated potential & possibilities opened by new material systems with reversible storage capacity.
- Experimental verification of the reaction of alanate destabilization with amides and of the reversibility of the process.
- Successful nano-sized metal powder precursor synthesis via the CVS technique.
- The Li_3AlH_6 + amide reactions are interesting, in that the PIs have demonstrated reversibility in Li_3AlH_6, whereas no other groups have been able to demonstrate this. However, these combined reactions are likely to produce a combination of the drawbacks of the two separate reactions: One reaction with an enthalpy that is likely too low (Li_3AlH_6) and another that is likely too high (LiH + amide).
- PI has presented a lot of interesting mechanistic results, but it seems that the results have not moved the hydride world much closer to surmounting the barriers and meeting DOE RD&D targets.
- The alanate-amide results show improvements, but the present thermodynamic and capacity properties seem little better than" many-year-old" doped nano-Mg (e.g., see Slide 19).
- At the 2006 Peer Review, there were worries about ubiquitous NH_3 emissions from amide systems. While PI has demonstrated NH_3 is apparently low enough to minimize cyclic capacity loss, this reviewer is disappointed that the absolute levels of NH_3 in the exit H_2 has not been yet quantified vis-à-vis PEM fuel cell tolerances.
- The efforts to synthesize nano-powders for the MHCoE are useful.
- Preliminary reversibility illustration of Li_3AlH_6 is a good result.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- Very strong coordination between this program and the remaining center activities. In particular, collaborations appeared to be developed for characterization experiments. Additionally, this program's CVS project supports center through supply of nano-powders.
- Substantial networking and collaborations with a good blend of expertise.
- Good to see this group quickly testing theoretical predictions, which can then either be pursued or discarded.
- This group's collaborations within the MHCoE seem outstanding.
- Recommend strong collaboration with SNL. They have extensive experience with amide systems. Poor collaboration with partners.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.7** for proposed future work.

- Future work scope should include reproducibility studies (especially in regards to reversible capacity) and purity determination and as stated, determination of the thermodynamic and kinetic properties for each reaction and reaction step. For the first reaction (Li_3AlH_6-$LiNH_2$), it is unclear why these experiments remain outstanding as it was 'future work' from FY06-07. Would encourage more collaboration with theoretical projects in center to help characterize current research as well as guide future work.
- Good to see intended continuation of support in regards to CVS synthesis of nano-powders.
- Materials selection is focused to alanate and amides. This question has been raised before and should be addressed. CVS synthesis of Li/Mg powders should be given more emphasis.
- The future plans are appropriate and justified by the experimental results produced so far.
- Not clear that the PIs have really good, novel creative ideas to build upon their previous results. They seem to be promising that they will continue working in the same area, but don't provide any details of how they will improve upon these reactions.
- This reviewer doubts that N-containing hydrides can be made to achieve DOE targets, but agrees with PI that it may be useful to continue keeping some amide work within the overall DOE program.
- The quantification of NH_3 should be given the high priority.
- The group's movement toward non-N systems may be wise.
- Work on CVS and high-pressure ball milling with help the MHCoE and should be continued.
- Reversible systems are important but energy efficiency is a key to on-board storage, focus should be perhaps redirected to other potentially less stable combinations.
- Recommend to clarify the purpose and show how rather known HEHP milling would help the synthetic efforts.

Strengths and weaknesses

Strengths
- The compositions and synthetic methods under investigation are relevant and promising. Additionally, the diverse set of characterization and property evaluation techniques that are in place are very valuable toward (further) clarifying the mechanisms and properties of storage materials.
- The PI is well-placed for the proposed work.
- Still exploring opportunities within the amides family.
- Good, solid collaboration record.
- The project serves as a useful contribution to the MHCoE.
- Overall good technical approach utilizing several characterization techniques.

Weaknesses
- The pace and degree to which the details (mechanism and properties) of each composition are being clarified is somewhat slow.

- The multitude of experimental techniques should be used collectively to confidently determine the reaction mechanisms. First-principles calculations should also be used to characterize existing and direct future research efforts.
- The PI does not like to change the emphasis related to materials.
- Release of ammonia is detrimental to the PEM fuel cells; it constitutes a significant drawback for amide-based systems and their use as hydrogen storage media.
- Work with amides has turned out to be problematical from a H_2 purity point of view, vis-à-vis PEMFC tolerance.
- Focus on higher stability systems/combinations is not considered.
- Concerns of ammonia formation and its measurement as a 1st step should be of higher priority.

Specific recommendations and additions or deletions to the work scope

- Quantify the ammonia concentrations involved and evaluate viability of material for storage applications - is it worth pursuing it as practical on-board hydrogen storage solution?
- There should be a go/no-go decision point for amide-containing systems during the next year, based on the upcoming NH_3 measurements. The level of NH_3 measured should be less than say 10 times what a PEMFC can tolerate. For example, if the PEMFC people require <1 ppm, then PI must demonstrate <10 ppm or ultimately abandon his systems.
- Alternatively, the project could accept the inevitability of unacceptable NH_3 levels and add a purification component.
- Recommend to shift focus to potentially less stable combinations.
- Confirm/measure ammonia formation as soon as possible.

Project # ST-22: Fundamental Safety Testing and Analysis of Hydrogen Storage Materials and Systems
Don Anton; Savannah River National Laboratory (SRNL)

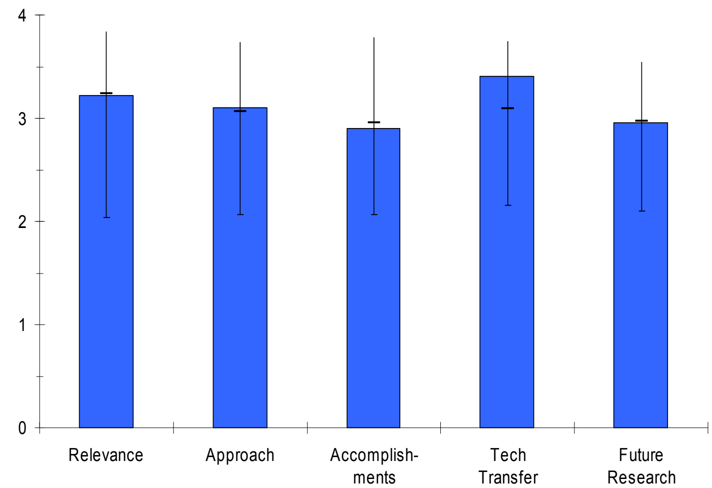
[NOTE: This project is not part of the Centers of Excellence; it is an independent project.]

Brief Summary of Project

The objective of this project is to fundamentally understand the safety issues regarding solid state hydrogen storage systems through:

- Development of standard testing techniques to quantitatively evaluate both materials and systems
- Determining the fundamental thermo-dynamics and chemical kinetics of environmental reactivity of hydrides.
- Development of amelioration methods and systems to mitigate the risks of using these systems to acceptable levels.

Overall Project Score: 3.1 (6 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.2** for its relevance to DOE objectives.

- This is a very important aspect of the program that has not been addressed.
- The outcome of the work should be used as a guideline for go/no-go decision on materials selection for all centers.
- Extremely important to pursue in parallel with development of new materials.
- Safe handling of hydrogen carriers/fuels is a major issue for the introduction of hydrogen-powered vehicles to the public. Therefore, projects that address this issue at any point during the supply chain will be an important determiner of which carrier should be used.
- Important point made by one member of audience: that on-board vehicle storage should also be included for greater fit with DOE objectives as at the moment the project appears more directed towards the mass transport of the carrier.
- Relevant to all metal hydride storage projects and other materials projects as well.
- Provides a safety program that will allow safety screening of materials, including novel/previously unknown materials.
- Quantifies or at least semi-quantifies safety.
- This project is critical for ensuring that systems can be developed for safely utilizing new hydrogen storage materials that meet DOE targets.
- Assessing the potential risks of solid-state hydrides and mitigating technologies/techniques is imperative.
- This work is premature given the intent of the project.
- Developing standards and codes when suitable materials have not yet been identified provides the danger of precluding materials that are otherwise interesting.
- There are no solid-state materials (other than the well characterized AB_2 and AB_5) that are suitable for automotive use. This kind of testing is overkill at this point.
- At this point a simple material MSDS and good engineering intuition will suffice for this stage of development.

Question 2: Approach to performing the research and development

This project was rated **3.1** on its approach.

- The current approach is good but needs to be expanded.
- Need to consider partially depleted materials.
- Need to address carcinogenic, mutagenic, respiratory, and in general toxicity of all potential storage materials.
- Good international partners and cooperation of tasks appropriate.
- Improvements could be made in process to ensure developments in H_2 storage materials are identified. Concerned that relying on attending conferences, H_2 storage committees, etc. is ad hoc, and would prefer to see more structured approach. However, understand this could be difficult.
- Maybe use checklist/database of materials that can be updated regularly. This could be an initial assessment of all the compounds currently under development with their evaluation status (whether the compound could meet the targets for commercial viability), i.e., under investigation, possibly viable compound, etc., with comments as to position in this project's analysis, i.e., if used in this project, why, and if not, why not analyzed?
- Generally believe they have identified most of the technical barriers although some more work could be done to understand the test standards for onboard storage and investigate mitigation requirements for this standard.
- Confused as to the pathway of the project. It may be helpful to provide/develop process showing potential outcomes.
- The project uses identification/mitigation methodology, which is very appropriate for safety studies (a "practice what you preach" approach).
- The actual series of testing methodologies include many proven processes.
- I especially like the methodology of mitigation testing and interaction with standards organizations.
- The technical approach is good and will systematically address key properties of the materials studied.
- The mechanism for ensuring that new materials emerging from other storage projects (and that are becoming prime candidates to meet DOE targets) are identified and provided to this project is less clear and will need some attention and support from DOE through the life of this project.
- They are not conducting tests that are performance related to automotive systems. A simple pyrophoricity test by dropping material in an air environment does not accurately describe how the material will react when packed into a tank in the case of a rupture.
- Additionally, containment methods today (pressure vessels) likely do not represent what will be used in the future, until we have identified suitable systems, I fear that most of this testing will become redundant or obsolete!
- They really need to collaborate with appropriate automotive safety groups, such as NHTSA, FMVSS and SAE to develop appropriate and useful test plans and procedures.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.9** based on accomplishments.

- Project relatively new so results limited.
- Have some quantitative data.
- Apparently have acquired equipment.
- Difficult to fully score here as only 10% complete after 2+ yrs although the project manager appears to have a reasonable understanding of the tasks and responsibilities – would expect greater % completion not sure if there were issues here that affected completion.
- Starting to get some good results – although it appears to be starting slowly (looking at the funding levels, it appears that this may be the reason).
- This is an ongoing process which should prove invaluable to materials testing and safety within the program.
- Showing some interesting thermodynamic pathway data. This will likely prove valuable.
- Good progress in the early project stages at the level of funding provided to date.
- Program has just started; but I don't see what novel work they will present.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.4** for technology transfer and collaboration.

- Via DOE program mangers, this project should be able to interact with other centers and independent projects to acquire safety and toxicity information.
- Fine team of international partners.
- Tied-in with IPHE.
- ICHS paper good.
- More could be done in terms of communication between partners to ensure that overlaps in undertaken research are reduced and so that each group could learn more from the other areas.
- Expect communication to improve and believe the idea given by the presenter for webshare would be a very good idea. Not sure of how regularly meetings are held but maybe also regular presentations via video conference or internet of each group's status and achievements could also prove useful within the group.
- Addition of regulatory body representation may provide useful advice on how the results of this project could be directed to a standard document – may also assist in providing structural focus to the research and mitigation strategy.
- Excellent international collaboration process – will greatly aid transfer of technical and safety data on an international basis.
- They need to ensure that lessons learned and safe practices methodologies are shared between participants.
- Very strong team of partners that also includes lead lab for the MHCoE.
- Participation of Sandia will help with identification and access to new materials being developed and as needed for testing but mechanism for such will need some attention.
- They have teamed with Dr. Fitchner of FZK in Germany, who has completed similar work in the past with guidance from OEMs.
- They really need to team further with OEMs when/if OEMs decide this work is ready to be conducted.
- They need to collaborate with appropriate automotive safety groups such as NHTSA, FMVSS and SAE to develop appropriate and useful test plans and procedures.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- Need to develop test matrix.
- Try to get fundamental relationships between quality of storage material and energy release.
- A matrix of the recommended test techniques for each of the storage materials relative to mass transport or on-board storage maybe a useful outcome for future. This may not be complete, but it may be a useful tool in identifying any gaps, etc.
- They are fairly early on in the process and still building.
- The path forward looks reasonable.
- I especially like the establishment of an internal website to share safety happenings/incidents, etc.
- This is a focused project with strong players and capturing the current knowledge base.
- Delay project until OEMs are ready and define what they need.
- Then team up with automotive safety related groups.

Strengths and weaknesses

Strengths
- Partners.
- Communication.
- Attempting fundamental understanding.
- Project is beneficial and required to assist in the safe market entry into hydrogen powered market.
- Strong international team.
- PI has much experience in this area.
- Well thought out approach/methodology.
- Dr. Max Fitchner.
- Technical expertise as represented by the PI and partners.

- Appreciation for need to develop sound and even novel technologies/techniques for risk mitigation associated with use of these materials.

Weaknesses
- Large scope.
- Probably underfunded.
- Ensure coordination among partners.
- Addition of industry and regulatory organization (codes & standards) advice may provide more breadth on risk mitigation perspective and industry introduction of standardized document.
- None that are obvious, other than things seem to be starting slowly – but looking at funding levels, this may be the reason.
- Path forward for interaction/collaboration with other storage projects less clear at this stage, but I am highly confident that this will be addressed by this team.

Specific recommendations and additions or deletions to the work scope

- This is a much-needed project that is long overdue to address the safety issues and metrics.
- It is recommended to increase the scope of this project to develop safety guidelines and targets used in down-selecting storage candidates.
- Currently this project appears underfunded. It is recommended to increase funding resources commensurate with scope expansion.
- Consider fire suppression techniques as part of task 3. Both lab, vehicle, and storage manufacturing scale.
- DOE should adequately fund.
- HSP should review safety plans for SRNL and UTRC and other U.S. collaborators – consider a site visit.
- Addition of industry and regulatory organization (codes and standards) advice may provide more breadth on risk mitigation perspective and industry introduction of standardized document.
- Review standards on onboard storage safety – on and off road vehicles.
- Matrix summary of status of each material and issues per material.
- Share learnings/best practices with the hydrogen community as a whole – via a website, maybe like h2incidents.org or similar.
- Per the discussion of Task 3 and the consequences of exposure-to-air and humidity for these materials, work on identifying and testing appropriate fire suppression agents for new materials should be considered.
- SwRI is serving as a testing laboratory for new materials coming from the Storage CoEs. Although their scope is different from this project, some interaction might be fruitful for both projects.

Project # ST-23: Hydrogen Storage by Reversible Hydrogenation of Liquid-phase Hydrogen Carriers [Official project title: Design and Development of New Carbon-based Sorbent Systems for an Effective Containment of Hydrogen]

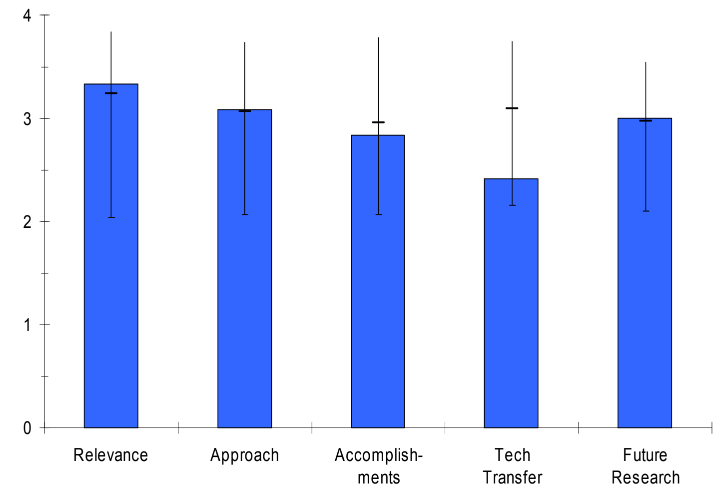
Alan Cooper; Air Products & Chemicals, Inc.

[NOTE: This project is not part of the Centers of Excellence; it is an independent project.]

Brief Summary of Project

This project is dedicated to the development of reversible organic liquid-phase hydrogen carriers for the delivery and storage of hydrogen. These liquid-phase carriers can be used to transport hydrogen from production sources, using the existing liquid fuels infrastructure, to sites where they can release hydrogen by dehydrogenation for stationary power applications or be dispensed to H_2-powered vehicles. The overall objective is the development of liquid-phase hydrogen storage materials with capacities of >7 wt. % and >60 g H_2/L and associated dehydrogenation and hydrogenation catalysts, and scale-up of liquid carriers for use in systems engineering activities as part of an associated DOE production/delivery project.

Overall Project Score: 3.0 (6 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

- This project attempts to develop a liquid hydrogen carrier that would have definite benefits for hydrogen on-board storage.
- Organic liquid carrier concept has real potential to become a viable hydrogen storage technology. The PIs are aware of the main challenges: lowering the temperature or heat input for desorption, improving catalyst effectiveness, and improving the capacity beyond the 7 wt.% "barrier". All of these will be non-trivial to overcome, but the PIs are working in the right directions.
- Having a (low-pressure) liquid fuel and liquid spent fuel is a significant advantage of this approach.
- Gravimetric performance is not close to the final target but this approach seems quite practical both for the on-board and off-board hydrogen delivery.
- Finding a high density liquid storage system with acceptable thermodynamics could significantly benefit the OEMs
- Finding a combined (exothermic/endothermic) system is an interesting approach to design systems with the appropriate systems
- The organic liquid hydrogen storage materials appear to have one of the best chances of leading to an H-storage system that meets DOE capacity targets.
- Air Products and Chemicals, Inc. (APCI) is making a concerted effort to identify and examine the most likely candidates.
- Lowering dehydrogenation temperature and carrier volatility are important longer range programmatic considerations.

Question 2: Approach to performing the research and development

This project was rated **3.1** on its approach.

- The approach seeks to develop novel, liquid-based hydrogen storage as a substitute for gaseous storage. The approach, while it must be considered high-risk, would have definite advantages particularly in terms of volumetric density of the storage system.
- Very effective use of combined experimental/computational approach. Should be used as an example for other projects, in this regard.
- APCI is also exploring a new auto-thermal on-board process.
- Autothermal process is an interesting idea that would help overcome the barrier associated with the high enthalpy materials. This idea should be pursued in the coming year, and next year it would be nice to see a bit more in terms of the overall energy efficiency of such an approach, and more specifics about the viability of such an approach.
- The approach considers using both on-board waste heat for dehydrogenation of the liquid carrier and an alternate autothermal configuration.
- New concept reflect to the biggest problem of chemical storage, how to get heat for dehydrogenation.
- The autothermal approach has the issues of reduced storage efficiency since some liquid carrier would be used for dehydrogenation heat and thus reduced volumetric and gravimetric densities. But may be required if there is not sufficient on-board waste heat from the fuel cell power system.
- While the combined exothermic/endothermic approach is commendable. I fear that the autothermal approach will bring us back to the point of on-board reforming systems. I highly doubt that they will be able to engineer a compact/efficient and cost effective system that meets our requirements.
- Storage and release of hydrogen in/from organic liquids with loosely bound hydrogen atoms is under study. The work involves identification of (1) organic liquids with suitable H uptake/release properties and (2) effective catalysts for the release process.
- APCI is investigating modified catalyst embodiments to improve dehydrogenation effectiveness.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.8** based on accomplishments.

- Good progress has been made in identifying and characterizing potential liquid carriers. Progress in the dehydrogenation of the various liquid carriers aided by catalytic additives was reported.
- A number of new liquid carriers are under study, including ones with >7 wt.% Hydrogen theoretical capacity.
- Several new concepts in the catalysis and thermal balance areas were reported on, but these are still works in progress.
- New concept of autothermal hydrogen release has been demonstrated that may help resolve the on-board storage efficiency issues, however, it moves the energy efficiency problem off-board (to the re-hydrogenation step) where additional "waste hydrogen" still needs to be put in the molecule that would be used on-board to compensate for the heat effect upon dehydrogenation. Another potential to reduce the efficiency problem would be to use other reducing agents (e.g., natural gas, etc).
- They have identified proven materials that work effectively in concert with each other to make the system work and provide the appropriate thermodynamic window.
- Better yet, the material combination is also taken into account for regeneration schemes.
- The only problem is that air is a required input.
- Given the funding level, the progress on this project has been modest in the past year. Earlier years seems to be filled with new results, new ideas, and new molecules.
- The presentation did not give a clear picture of the amount of real progress towards an operating system over the past year. A graphic showing how the program is moving towards its end-state goals on an annual basis might help clarify this.
- There is less than a year left for this project and over $6M will have been spent. It doesn't seem that APCI will come very close to meeting the original expectations of the program. Will we have a liquid carrier that can meet at a minimum the "system" capacity targets for 2010?

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.4** for technology transfer and collaboration.

- There appears to be little collaboration on this project, perhaps due to the proprietary nature of the work at Air Products. However some collaboration with ANL was mentioned and input was requested from the auto OEMs.
- Not clear that this project is significantly interacting with any other projects. It could be interesting to see a more substantial interaction with one of the automakers, for instance.
- Typical Air Products – not much collaboration. But then again, they really don't need it; they have excellent resources in-house for the job.
- There doesn't seem to be any meaningful collaboration outside APCI.
- It is not clear to this reviewer why this project is not more closely connected with, or even an actual part of, the Chemical Hydrogen CoE.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- Presentation ST-31 reported a compensation factor of about 1.6 for gravimetric material H-storage capacity for organic liquids compared to system gravimetric capacity. That means the 2010 goal can be achieved for a liquid with H-storage capacity around 10 wt.%. In light of this, it seems prudent for Air Products to focus their attention on compounds that have a chance to deliver at least 9 wt.% H. There seems to be little point to experimenting with compounds that can't at least in theory release 9 wt.% H.
- Highest priority emphasis should be on identifying liquid carriers that can meet H-storage targets.
- Considerations related to releasing all of the theoretically available hydrogen should follow the above.
- Issues related to release temperature, energy balance, and volatility should come after that.
- Catalyst research is also necessary to pursue for potential improvements of system weight and volume and kinetic characteristics.
- Autothermal dehydrogenation has a potential to resolve major energy efficiency issue on-board
- At the same time, search for new carrier(s) with lower dehydrogenation enthalpy is also necessary to improve overall efficiency
- Please find away to eliminate any outside inputs such as air or water; this complicates the reactor significantly in terms of after-treatment.
- The project was reported to be 75% complete at this point. Future plans for the remainder of the work seem to be reasonable, but a lot of work is needed to fully evaluate the full potential for liquid hydrogen carriers.
- Future work is focused on the most critical barriers; however, the plan to overcome these barriers is not clear. For instance, improved catalysts are certainly needed, but how do the PIs propose to find them?

Strengths and weaknesses

Strengths
- Use of hydrogen carriers for both on board and off-board applications.
- Improved safety as compressed hydrogen is not utilized.
- There is a potential to overcome on-board storage efficiency issues with the autothermal dehydrogenation approach.
- Novel ideas (unlike other projects in portfolio).
- Liquid fuel (could use conformable tanks).
- Great combined use of experiment/computation.
- This is a very innovative concept from a practical point of view.
- Novel.
- Functional.

Weaknesses
- Relatively small progress being made towards the discovery of new carriers with increased capacity and reduced enthalpy of dehydrogenation.
- System start-up and transient response may be serious issues to resolve on the system development stage.
- Capacities for these molecules (at least for low enthalpy) appear to be significantly limited by H:C ratio.
- Progress in this project was initially quite fast, but seems to have slowed recently.

- Material seems solid in the low room temperature
- Autothermal concept requires air!
- APCI seems to be working alone in this project. What has prevented the development of close ties with related projects in the Chemical Hydrogen CoE?

Specific recommendations and additions or deletions to the work scope

- None.
- A decision on whether or not to pursue the autothermal approach should be made as soon as possible in order to focus the remaining effort. Suggest that emphasis should be on selecting a specific liquid carrier and fully characterizing the dehydrogenation and regeneration of the selected carrier.
- The PIs should be encouraged to try and demonstrate this autothermal concept; it could potentially remove one of the significant barriers associated with this approach.
- See recommendations in the "comment" boxes above.

Project # ST-24: DOE Chemical Hydrogen CoE Overview
Bill Tumas; Los Alamos National Laboratory (LANL)

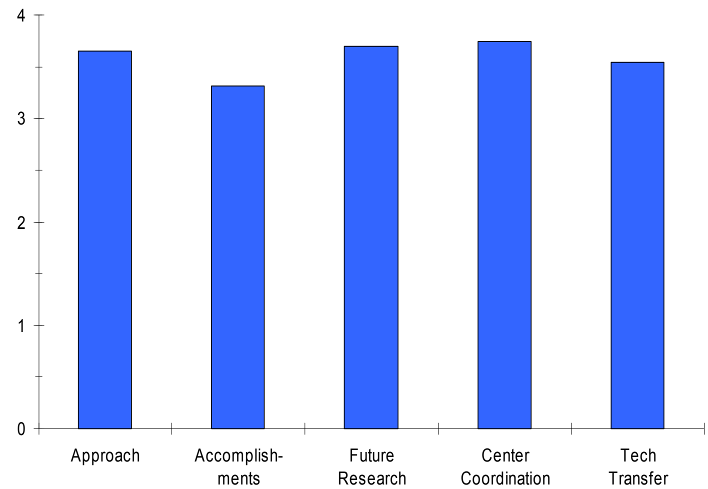
[NOTE: This presentation was to evaluate the entire Chemical Hydrogen Storage Center of Excellence as a whole. A separate review form was used and can be found in Appendix D**.** LANL's technical contribution to the center is evaluated in ST-29. **]**

Brief Summary of Project

The Chemical Hydrogen Storage Center of Excellence (CHCoE) involves two national laboratories, seven universities, and four industrial companies. The objectives of the center are to identify, research, develop and validate advanced on-board chemical hydrogen storage systems to overcome technical barriers and meet 2010 DOE system goals with the potential to meet to 2015 goals:

- Develop materials, catalysts and new concepts to control thermochemistry and reaction pathways;
- Assess concepts and systems using engineering analysis and studies;
- Select most promising chemical systems for engineering development.

Overall Project Score: 3.6 (6 Reviews Received)



Question 1: Approach to performing the R&D

This project earned a score of **3.7** for this criterion.

- Center very well organized and focused on challenges.
- Aimed squarely at the barriers and well designed for partner strengths. Clear go/no-go structure and internal goals. Fairly diverse set of approaches now.
- Strong management team.
- Important that the center is actively stopping work (down select process) on materials that don't show potential, so scarce resources is not wasted.
- Generally, I like the management structure and approach. Although reactor engineering is part of their future plans, I would appreciate seeing upfront calculations using a template material, rough engineering, and a cost study to see if there are any obvious show stoppers. This could also be used to help set qualitative practical targets for regeneration, storage, and hydrogen release.
- Pathway to promising advanced technologies as well as borohydride and ammonia borane is considered in this CoE.
- The scope of the center is largely limited to boron chemistry. Boron is light element, abundant enough in nature that demonstrates very rich chemistry. This opens the door to a variety of ways for storage and regeneration. At the same time little effort is devoted to exploratory advanced concepts other than boron.

Question 2: Technical accomplishments and progress toward DOE goals

This project was rated **3.3** for this criterion.

- Aminoborane work shows excellent progress to overcoming key challenges and targets.
- Establishment of regeneration process from spent fuel should be accelerated as well as system study for hydrogen generation to clarify requirement to material properties.

- Significant progress has been made toward goals, but there is still much to do. Spent fuel regeneration is moving along. Some systems have been taken to a point where they are sure there is no need to go further. MBN systems are a good addition. Adding combinatorial catalysis system is also a needed ability.
- If the data are available, I would like to see some overall yields for the forward and reverse reactions to assess the overall cycle efficiency.
- Still, a lot of technical barriers exist to be overcome that are associated with boron ranging from use and regeneration of $NaBH_4$ to kinetic issues of H_2 release from and regeneration of ammonia boranes. Perhaps, a go/no-go decision on $NaBH_4$ can be facilitated based on both on-board operability and off-board regeneration efficiency issues. (Note: DOE's go/no-go decision on $NaBH_4$ in FY07 will be facilitated based on both on-board operability and off-board regeneration efficiency).

Question 3: Proposed future research approach and relevance

This project was rated **3.7** for this criterion.

- Good focus on exploratory / innovative research to invent new materials and concepts.
- Down-selecting the best materials and continuing to pursue elements with high (2+) hydrogen release rates should maximize the results of this CoE.
- The timing for materials down-select process is reasonable for the DOE target dates.
- Seems like a suitable plan though the backup plans, as with all centers, seem scant.
- It isn't clear if focus should be on improving efficiency of regeneration schemes for AB until a go/no-go decision is made.

Question 4: Coordination, collaborations and effectiveness of communications within the CoE

This project was rated **3.7** for this criterion.

- Excellent communication within the CoE is apparent.
- Based on the information provided, coordination and collaboration appears to be very good.
- The CoE considers correlation with other CoEs well.
- The CoE promotes "Engineering Assessment and Coordination Crosscuts Center Activities" for better cooperation between engineering and scientific research.
- Coordination and communication seems largely good. There are still some players (at the poster session) who seem adrift doing their small sub-segment and just counting on someone else to make whole system work without even really knowing what that entails; but generally communication is good.

Question 5: Collaborations/Technology Transfer Outside the CoE

This project was rated **3.5** for this criterion.

- As material selections from other CoEs converge, more communication between the CoEs will be crucial to ensure work is not being duplicated/repeated.
- The CoE have tried to expand the possibility of chemical hydride by means of collaboration with researchers in foreign countries through the IPHE framework etc.
- All centers could do this more, but there is communication, it could be significantly more frequent and addressed with greater intent to benefit the overall program. Metal Hydride CoE and Chemical Hydrogen Storage CoE are working together on alane now. Organic chemists are exchanging ideas across teams.
- Although not clear from the presentation, the Q&A uncovered interactions between this CoE and the CoE for metal hydrides.

Strengths and weaknesses

Strengths
- The network with foreign researchers through IPHE.
- Strong leadership is apparent in the progress being made at this center.

- Strong management across the whole center.
- Right team for the area. Good management model.
- Good approach to center project management.
- Technical issues appear to be well understood.
- The CoE is flexible to change as the down-select procedure narrows the group of potential materials.
- Innovative ideas and healthy pipelines of new candidates.
- Excellent combination of theory, experimental, and system cost/analysis.

Weaknesses
- Still very dependent on BO to BH chemistry, and while a quite interesting approach to this is being worked out it is far from a sure thing, so further diversification would seem a good course.
- Probably would benefit from actual collaboration with Production/Delivery team because this system has the added need to return spent fuel to the maker.
- Would like to see more upfront cost analysis and to use this information to qualitatively set some of the technical targets.
- Although it does not really fit into this category, I felt that the presenter had too many slides and the presentation was rushed. I would suggest narrowing the range of topics covered and focus more on high level messages.

Specific recommendations and additions or deletions to the work scope

- Center members seem to have different visions of appropriate efficiency. This should be uniform.
- Materials that meet the requirements for on-board operations can be down-selected for dedicated regeneration studies, as opposed to addressing regenerability issues for majority of the materials under investigation.
- Good approach for analysis and selecting optimal regeneration process has been demonstrated by Rohm & Haas that could be applied towards material selection for storage as well.

Project # ST-25: Novel Approaches to Hydrogen Storage: Conversion of Borates to Boron Hydrides
Suzanne Linehan; Rohm and Haas

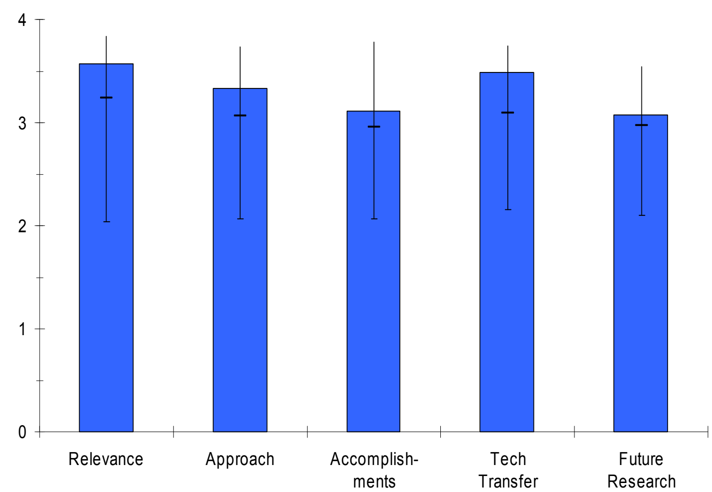
[Member of the Chemical Hydrogen Center of Excellence]

Brief Summary of Project

The overall objective of this project is to define and evaluate novel chemistries and processes to produce chemical hydrogen storage materials that meet DOE 2010 targets, and that have the potential to meet 2015 targets.

- The primary focus is to identify energy efficient and cost-effective options for B-OH to B-H conversion.
- A secondary objective is to leverage Rohm and Haas' expertise and experience across the entire center, assessing engineering requirements, economics, and life cycle inventory of hydrogen storage materials other than borohydride.
- A third objective is to support DOE's Chemical H_2 Storage Systems Analysis Working Group.

Overall Project Score: 3.3 (7 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.6** for its relevance to DOE objectives.

- Consistent with President's Hydrogen Fuel Initiative.
- The lessons learned in this program represent a valuable contribution to the DOE's Hydrogen Program.
- Important to the chemical hydride effort in DOE's Multi-Year Research Development & Demonstration plan by carefully examining the technical and economic aspects of $NaBH_4$ regeneration from spent borates (i.e., after the Millennium Cell on-board hydrolysis process).
- Presentation addressed broadly, but very well, the goals of the national initiative.
- This exhaustive (dragnet) approach to determining all possible $NaBH_4$ regeneration methods is absolutely necessary to put true closure on the question of the feasibility of economically viable $NaBH_4$ regeneration.
- A stipulated overall objective for this program is to examine chemistries that can meet the 2010 and possibly the 2015 H-storage system targets set by DOE. Rohm & Haas has done an admirable job of assessment, analysis, and experimentation on the $NaBH_4$ system as a hydrogen storage material. All indications at the present time are that it will barely meet the 2007 targets. In short the SBH system is at best a test case for the boron-based materials and for slurry type approaches.
- Necessary to do this sort of analysis to sort out the possible efficiencies for $NaBH_4$ regeneration.
- Probably the critical challenge for these systems is recycle energy and engineering the system.

Question 2: Approach to performing the research and development

This project was rated **3.3** on its approach.

- Good focus and start on quantifying the thermodynamics and cost of $NaBH_4$ regeneration from spent borates.
- Thermodynamic modeling followed by experimental confirmation is an excellent approach and greatly needed by DOE for the go/no-go decision on $NaBH_4$ hydrolysis.
- PI and collaborators have competence and skill in attacking this long-standing regeneration problem.
- Very professional presentation and analysis of the project.

- Experimental and theoretical approach – very well described.
- Plan, etc., were very well presented. Efficiency analysis was similarly well documented.
- Paper study of approximate energy is appropriate. Metric for overall weighting is arguable (everyone has their own weighting) but useful.
- Excellent that as many different routes and chemistries were considered.
- Weighting system seems a bit arbitrary (as is inevitably always the case) however it seems reasonably well aligned with DOE's goals.
- Why an internal regenerating efficiency of 60%, FreedomCAR/DOE targets are higher.
- The work involves finding a cost-effective way to convert borates to boranes. The tasks cover literature searches, screening and evaluation, development of flow sheets and cost estimates, and laboratory demonstrations of key process steps.
- The approach taken in this program has been well thought-out from the beginning. The problem is that the H-storage "system" targets are set at a high level and very few H-storage material concepts have a chance of meeting them.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.1** based on accomplishments.

- R&H has done an excellent job of scoping and evaluating the regeneration options. The respective options have been examined in considerable detail, quantified, and ranked in a sensible way.
- Judging from this presentation and related $NaBH_4$ presentations and posters, it is clear that R&H is making an honest, forthright effort to put $NaBH_4$ technology in proper perspective.
- Excellent and exhaustive work conducted (literature study).
- All obvious regeneration processes have been studied in detail, at least on paper. Good presentation. Moving well toward the one intent of the project, namely to help DOE in making the go/no-go decision on $NaBH_4$ hydrolysis.
- Results are likely to be very useful for the go/no-go decision.
- Weighting factors of the various contributions seem to be somewhat "underweighted" on the environmental/CO_2 impact of the regeneration strategy. This leads to some skepticism of the final ranking of the regeneration processes.
- Group has determined that metalothermic reduction is the most promising regeneration route. This is consistent with Prof. Suda's conclusions of the last few years. Why was that Japanese work not cited? Does PI think Suda's projection of $2/kg $NaBH_4$ is possible?
- Other possibilities quantified.
- Important cost projections not quite ready. These are needed soon and will be critical.
- Details were not really provided in the presentation except for the various projections and feasibility analyses.
- Clearly, the results are positive for the metal hydride and metal reduction routes to regeneration.
- Provided some lab evaluations such as the metal based regeneration of boron wastes. Generated information to set rankings and ranked the efforts. Paths elucidated and energy, complexity, etc. evaluated. Seems like perhaps more might have been accomplished on a largely paper study with this budget.
- Would like a little bit more validation by real world results or studies (perhaps also obtained from literature).
- The calculations done seem quite simple, and it's not clear why such a large amount of funding was necessary to produce these results.
- Does not appear as though they have delivered on the milestones promised in Q1 FY07 (still listed as "ongoing").

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.5** for technology transfer and collaboration.

- Excellent.
- Excellent collaborations and tech transfers through the CHCoE.
- Excellent collaboration with CoE partners.

- Other services beyond $NaBH_4$ useful to the CHCoE.
- Interacting well as center partner.
- R&H has a set of collaborations within the CHCoE that support and augment their effort in meaningful ways.
- Perhaps their collaborations will lead them to a new or at least revised direction that has a better chance of meeting storage targets than $NaBH_4$.
- Why are there no collaborations with Suda/Japan?

Question 5: Approach to and relevance of proposed future research

This project was rated **3.1** for proposed future work.

- The cost estimates are really a critical contribution, and will be necessary for an informed go/no-go decision. Thus, this work should be completed ASAP.
- Very nicely consistent with past results and very well focused toward the $NaBH_4$ regeneration barrier.
- This reviewer (and presumably DOE) is anxious to get some cost estimates for regeneration.
- This is based on a series of excellent analyses.
- Appropriate.
- Please add some extra calculations as to what further inefficiencies occur with removal/pumping and shipping the fuels from the vehicle, to fueling/reprocessing plants.
- The R&H path in the future will depend on the outcome of work over the next few months. In the short term, they need to pour their efforts into putting their $NaBH_4$ technology in the best possible light. The outcome of the go/no-go decision process will determine how they proceed beyond September of 2007.
- In parallel with the $NaBH_4$ work, they should work with their CoE collaborators to define a follow-on path for their storage work if $NaBH_4$ is discontinued or modified in scope.
- Amino-boranes may be the way to go in the future. Systems with a ratio of H to other atoms equal to or greater than 2 seem to be the most promising.
- Not exactly clear what actual chemistries they will try to validate or why? Their results show that there is no route that is sufficiently energetically efficient to meet their own criteria, let alone the more stringent DOE Criteria.
- Not completely clear what will become of this project. Should there be a "no-go" decision on $NaBH_4$?

Strengths and weaknesses

Strengths
- This is a nicely detailed and directed effort on $NaBH_4$ regeneration. It is much needed.
- The people involved are with industry and are experts on process thermodynamics and economics.
- The process for the down select is clear.
- The presentation suggested very high levels of competence in the project and in the study participants.
- Well-planned and justified series of projects and emphasis for the future.
- Honest conclusions about challenge to these regeneration schemes.
- A strong team with dedicated personnel.
- Appropriate resources to contribute to the hydrogen storage program in an effective way.

Weaknesses
- At the technical level, this project has no obvious weaknesses. R&H is doing all they can to bring borate recycle to a demonstration. They are limited by what the system is capable of in terms of storage capacity, functionality, and cost.
- They need to make some significant progress over the summer in borate to borane conversion to make a convincing case that regeneration can be accomplished at an acceptable cost.
- Processes in which CO_2 is evolved need to be considered with respect to concern about greenhouse gas emissions.
- Intuitively, the difficult thermodynamics of regeneration pose a major challenge. This reviewer has always doubted that this will result in H-storage cheap enough for vehicles. But, by all means, good luck.
- Few actual results were presented.

- The calculations done seem quite simple, and it's not clear why such a large amount of funding was necessary to produce these results.
- Why are there no collaborations with Suda/Japan?

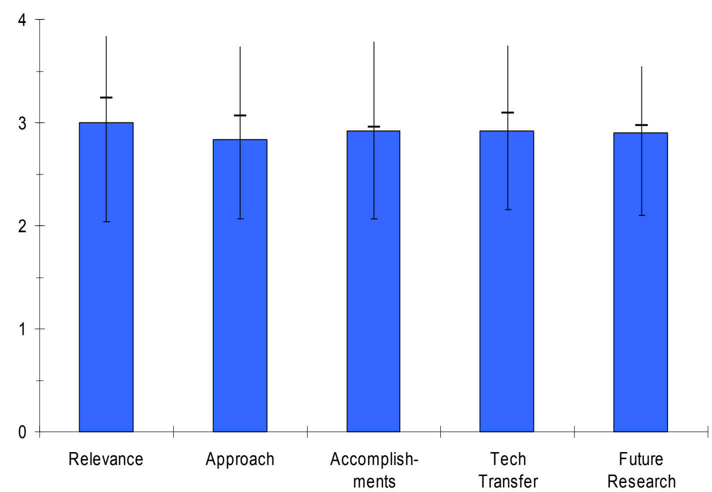
Specific recommendations and additions or deletions to the work scope

- No significant overall change is recommended.
- Suggest making use of prior thermodynamic and experimental work by Suda on metalothermic reduction; optionally consider establishing collaboration.
- Down select shall be done with the absolute cost/price potential, I hope the figure will be shown with the related analysis.
- None, except possibly more time for the work.

Project # ST-26: Electrochemical Hydrogen Storage Systems
Digby Macdonald; Pennsylvania State University

[Member of the Chemical Hydrogen Center of Excellence]

Overall Project Score: 2.9 (6 Reviews Received)



Brief Summary of Project

Two strategies are pursued in this Pennsylvania State University project to advance hydrogen storage technology. In the first case, hydride hydrolysis/ regeneration is investigated by exploring the electrochemical reduction of B-O to B-H, while in the second strategy the electrochemistry of various polyhedral boranes is explored to ascertain if electrochemical transformations can be affected between various members that reversibly absorb and release hydrogen and hence could form the basis of a new hydrogen storage technology.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.0** for its relevance to DOE objectives.

- Consistent with President's HFI.
- Regeneration of sodium borohydride can be done either chemically or electrochemically. PSU is looking at electrochemical routes to regenerate sodium borohydrate (borate to borohydride). The project is highly relevant to the mission of the CHS CoE particularly to $NaBH_4$ regeneration.
- This work fits in with the other $NaBH_4$ efforts to help determine whether electrochemical regeneration of $NaBH_4$ is possible.
- Adds to the chemical hydride effort in DOE's Multi-Year RD&D plan by looking at electrochemical methods of $NaBH_4$ regeneration from spent borates.
- Clearly the regeneration of $NaBH_4$ is key to this overall process.
- This will determine the future of this (hydrolysis) program.
- The results, if achieved, will ensure the success of the initiative.
- This project is examining a possible spent fuel regeneration route for the $NaBH_4$ process. A near-term advance in this area could save the day for $NaBH_4$, which is approaching a go/no-go decision point.
- The main concern here is can the project deliver in time to impact the go/no-go decision.
- Why work on electrochemical regeneration when Rohm & Haas work clearly demonstrates that energetically it is one of the least efficient and most difficult?

Question 2: Approach to performing the research and development

This project was rated **2.8** on its approach.

- Electrochemical hydrogen storage is a relatively unexplored idea, and hence the present effort is interesting; however, the PIs need to clarify the overall energy balance of such an idea. How much energy input is required in a typical electrochemical process in order to extract the hydrogen?
- One project focus is on electrolytic regeneration of $NaBH_4$from the spent borate resulting from hydrolysis. Also covered in part by the Rohm & Haas presentation (ST-25). That is important to the DOE $NaBH_4$ hydrolysis go/no-go decision DOE must make in FY2007.

- Project also looks at electrochemical H-storage in the polyboranes, an area that has not been heretofore covered in the DOE program.
- Clear success in either will help toward breaking down H-storage barriers.
- Impressed by the approach.
- Developed a technique for identification of BH_4 in product.
- Addressed the low electrochemical yields and problems of reproducibility.
- Investigator takes a very realistic approach to the studies and the results.
- PI clearly recognizes the problems of this 8e- reduction.
- The approach is based on electrochemical and plasma chemical methods that are clearly promising but at the same time high-risk in nature.
- Success requires winning boron form an anionic moiety – not an easy thing to do, but the PI has ideas that just might work. At least they deserve some feasibility testing.
- The approach is focused on the technical barriers to efficient regeneration.
- The approach could be strengthened by assessing the feasibility of chemically assisting the electrochemical reduction reactions.
- Really trying to work against "Mother Nature" by forcing a negative ion to a negative plate!
- It is difficult to imagine how a system deliberately intended to work against thermodynamics and forces will ever lead to high yields and efficiencies.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.9** based on accomplishments.

- Some initial success of electrochemical regeneration pathways for $NaBH_4$.
- Some experiments give hints of BH_4^- generation, but clear promise is not convincingly shown.
- The development of the needed electrochemical testing techniques is apparently successful and complete.
- The potential for reversible electrochemical H-storage is not yet convincingly shown.
- Achieved the "in situ" method for BH_4 detection.
- Made progress toward understanding the process occurring at the electrode [use of (Et4N)OH].
- Obviously the progress made is not very substantial in reaching the goal but the direction is right on-target.
- Given the challenges, he has demonstrated excellent progress.
- The literature has been well reviewed and a variety of electrochemical deposition tests using alternative electrode materials and electrolytes have been performed.
- Reasons for the discrepancies in the literature concerning electrolysis of the borate anion have been sorted out, but attempts to actually produce boron in a reduced state have been only minimally successful.
- A quantitative method to determine borate in aqueous solution was developed during the past year.
- Development of the analytical technique electrochemical reduction of B-O to B-H was demonstrated.
- The electrochemical activity of polyboranes has been investigated.
- Multiple redox transitions were discovered in polyboranes.
- Given the project has been in place for more than two years, progress toward breaking technological barriers is not certain.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.9** for technology transfer and collaboration.

- Good collaborations with Rohm & Haas, Millennium Cell, and the CHCoE.
- Collaboration appears strong between PSU and other center members.
- Good collaboration with several members of the CoE.
- This project is directly supporting the Rohm & Haas $NaBH_4$ program. It is addressing an issue that seems singularly important to $NaBH_4$ regeneration at this time.
- Perhaps work on the polyboranes will lead to a new research direction even if $NaBH_4$ faces a no-go in September.

- The PI is a world class electrochemist. Surely, there are opportunities for applications of his expertise within the other CoEs for H-storage.
- Minimally involved with others, although R&H and LANL are good partners.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.9** for proposed future work.

- Need to demonstrate reversibility of electrochemical storage, and also give an indication of the energy efficiency of such an approach.
- Reasonable future effort on B-O to B-H electro-conversion. The problem is the limited time frame until the DOE go/no-go decision point.
- Electrochemical studies will build on the very important "early" results obtained.
- Presentation implied that the investigators are moving slowly, but correctly, towards the goals of the project.
- The proposed ideas about how to electro-reduce borate are deserving of study.
- Focus for 2007 is on overcoming electrostatic repulsion of $B(OH)_4$ from the cathode in the electrolysis cell.
- Another task will look at chemical reduction by means of hydrogen plasma.
- The electrochemical H-storage polyborane half is reasonable.
- The polyborane work might open new windows of opportunity for borate utilization in fuel cells.
- Not exactly sure what his next intended steps are.
- Not clear what will become of this project in light of the upcoming go/no-go decision on $NaBH_4$.

Strengths and weaknesses

Strengths
- Project supports $NaBH_4$ regeneration effort.
- Reversible electrochemical storage successes would offer an exciting new option.
- Competence of the investigators.
- Addressing of the drawbacks of the problem of repulsion of the meta-borate anion by the electrode.
- The PI is an expert in the field of electrochemistry and has a broad range of research experience that could be gainfully employed throughout the HFCIT program.
- The research infrastructure at Penn State is first class for the kind of experimentation required to achieve success in this project.
- Good understanding of the electrochemical pathways to successfully regenerate B-O to B-H.

Weaknesses
- The inherent thermodynamic difficulties of B-O to B-H conversion. Regeneration must be of very low cost (maybe < \$2/kg $NaBH_4$ regenerated) to be applicable to vehicles.
- Difficulty of the electrochemical regeneration.
- Working against thermodynamics!
- The project may be too narrowly focused on the addition of H to B-O. Another possibility is to remove O from B-O.
- The main concern is that there is not much time left to show a truly encouraging result for the borate reduction. Hopefully, the team at Penn State plans to run full bore this coming summer.
- In truth, the chances of success in achieving efficient borohydride regeneration are not great, but it is worth a try.
- Lack of overall progress.

Specific recommendations and additions or deletions to the work scope

- PSU should consider molten salt processing of B-O bonds and/or removal of O from the borates rather than the addition of H.
- Add nuclear power and renewable energy options to the list of electricity sources that complement the electrochemical approach to $NaBH_4$ regeneration.

- Add a go/no-go decision point in the next year to the effect that at least some reversible electrochemical H-storage must be demonstrated.
- Cease all B-O to B-H regeneration work if DOE decision in FY2007 is no-go.
- At this point, it seems that the investigators will require more time.
- Go full bore on the borate reduction work in the near term.
- The center and PSU should develop a detailed plan that maximizes the amount of information that this approach can bring to the go/no-go decision process.
- Recommend that this work be moved into the BES portfolio.

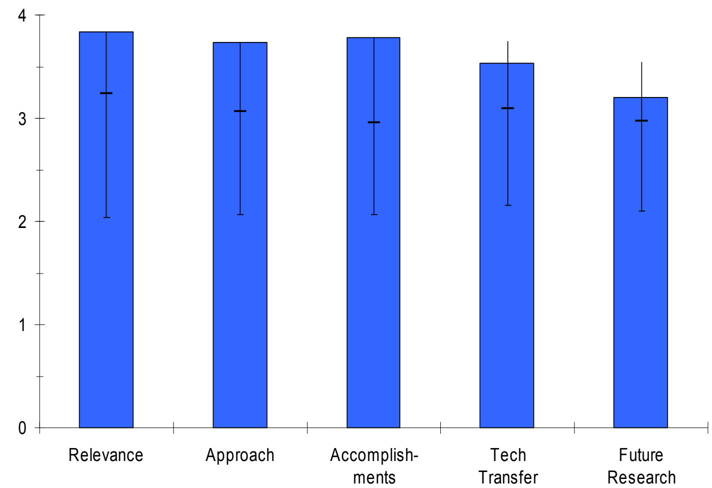
Project # ST-27: Amineborane Hydrogen Storage
Larry Sneddon; University of Pennsylvania

[Member of the Chemical Hydrogen Center of Excellence]

Brief Summary of Project

The objectives of this project are to:
• Develop methods for on-demand, low-temperature hydrogen release from chemical hydrides that can achieve DOE targets.
• Develop high conversion off-board methods for chemical hydride regeneration.
Also, in collaboration with center partners the goal of this project is to develop new methods for amineborane hydrogen-release and regeneration reactions that will enable their use for chemical hydrogen storage.

Overall Project Score: 3.7 (6 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.8** for its relevance to DOE objectives.

- Because of the potentially large theoretical hydrogen capacities of the amineboranes, they are important candidate materials to achieve the 2010 storage targets.
- Program addresses important questions for hydrogen storage in chemical systems that show promise for meeting system goals.
- Use of ionic liquids as a method to both liquefy aminoborane (AB) and improve kinetics and capacity is necessary and novel.
- Work impacts specifically to high capacity storage materials, e.g. amine boranes.
- Project is relevant to DOE objectives.
- As part of the CHCoE U. Penn is studying amine borane chemistry, specifically thermal and catalytic dehydrogenation of AB and the reverse, rehydrogenation. The work aligns well with the DOE program objectives, and is a critical part of the center activities.

Question 2: Approach to performing the research and development

This project was rated **3.7** on its approach.

- Amine boranes could meet DOE targets. Thermally induced dehydrogenation of AB is known to be very slow at temperatures of interest. Therefore, the approach is focused on discovering a catalyst(s) to increase the extent of hydrogen release at appreciable rates at temperatures of interest, which addresses the DOE weight and volume barriers.
- This project has an excellent focus on the problem areas, and excellent concepts to address the problem areas.
- Liquid amineboranes may be promising new materials approach.
- Hydrogen release from ammonia borane using ionic liquids and metal catalysts is an extremely promising idea.
- Excellent use of ionic liquids with addition of metal hydrides and proton sponges.
- Good approach looking at a number of different chemistries of amine boranes focused on getting the best performance, mainly kinetics.
- Address kinetics and system energy density issues.

- Have a good understanding of the chemistry, demonstrated by the identification of undesirable side-products formed in the AB-LiH or $LiNH_2$ systems and their early move from these to strong N-bases to aide the elimination reactions.
- Good self-regulating down select approach. PI does good job at evaluating progress on a given chemical system, and explores alternatives rapidly.
- Have implemented no-go decision on hydrolysis of ammonia triboranes after determining it can't meet 2015 goals.
- Addresses spent fuel regeneration and have developed an approach that bypasses borates, which should lead to lower energy demands for regeneration.
- They are also identifying novel, low-energy methods for regeneration.
- Off-board regeneration of ammonia borane: major problem in the field. Approach proposed is a good starting point for the future work/further development.
- The use of solvents does take a toll on both the gravimetric and the volumetric capacities of the amineboranes.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.8** based on accomplishments.

- Showed significant improvement in H_2 release from ammonia borane systems
- On a material level, has exceeded 2007 targets for volumetric density and gravimetric density and appears to have met 2010 targets with one system (but need better kinetics).
- Have made significant contributions to understanding of the mechanism of the H_2 elimination reactions in these systems.
- By far, some of the best progress and novel ideas in the entire hydrogen storage program.
- Good progress in looking at various alternatives for getting rapid kinetics at target temperature (85°C). Completed studies of a number of different amineboranes systems.
- In 2007 several additional ionic liquids were found that increased the number of equivalents of H_2 released from around 1 to a little over 2.
- The gravimetric density increased to 7 wt.% at 85°C and the volumetric density to 0.039 kg/L.
- Promoters increased hydrogen release from solid AB to 9.5 wt.% but released NH_3, an undesirable byproduct. Use of proton sponge avoids the formation of NH_3 and is a significant accomplishment.
- Triborane alone has capacity limitations, but may be used in combination.
- Ionic liquids have capacity limitations.
- Chemical promoters ($LiNH_2$, LiH), mixtures of AB and AT, proton sponge have been studied.
- Excellent experimental work overall.
- Very interesting results on hydrogen release.
- Hydrolysis has been de-emphasized due to the associated regeneration problems.
- Thermolysis still has a significant problem with the rate of hydrogen generation.
- A new regeneration process was developed that avoids the formation of B-O bonds. These are significant accomplishments and represent substantial progress since last year.
- A potentially important new regeneration route for thermolysis reaction products has been identified.
- Have demonstrated a new process for ammonia borane regeneration.
- Regeneration: multi-step process; cost efficiency is low; complexity is high; a good chance that it may be not scalable.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.5** for technology transfer and collaboration.

- Very extensive collaborative efforts to support various aspects of the approach.
- Collaborations with others in the chemical hydrogen storage center are evident.
- Working with all the appropriate partners in the center.
- Good collaborations within CHCoE.
- Appears to be very interactive with center members.

- Collaboration with other research and industrial partners is very good.
- Collaboration and sharing of information is evident across the Center.
- PNNL and LANL will develop engineering assessments of both liquid and solid systems and regeneration processes.
- Rohm and Hass will also perform an engineering assessment and scale-up of the new regeneration process.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.2** for proposed future work.

- UPenn will continue to develop and optimize chemical additives to improve hydrogen release rates.
- UPenn will work with center partners to define and optimize the new AB regeneration process.
- Good exploration of alternatives for the amineborane system.
- The plans follow the results of past work in a logical progression.
- Proposed future work appears to be an extension of current work.
- Improving the release rates of the thermolytic aminoboranes is a key issue.
- Regeneration of boron-based materials deserves even more attention.
- Technology transfer issues for the regeneration process of the thermolytic aminoboranes are key issues. Will it be cost and energy efficient?
- Future work is formulated in very general terms.

Strengths and weaknesses

Strengths
- Have a good understanding of the underlying chemistry.
- Good understanding of the chemistry involved.
- Very strong chemistry approach.
- Innovative ideas.
- Have focused on chemistry and systems that can meet the targets.
- Have made significant progress in spent fuel regeneration and in improving kinetics and amount of H_2 release.
- Ability to explore chemical systems fairly rapidly and maintains focus on relevant properties.
- Extensive collaboration.
- Very solid experimental work.
- The project is really focused on achieving the DOE targets. Several materials and processes have been abandoned when it became evident that they did not have the potential to meet the targets.

Weaknesses
- None.
- It is still not quite clear how regeneration of the used ammonia borane could become economically feasible.
- The reduction in release rate after the first equivalent of H_2 is released is an issue.
- Ionic liquids have capacity limitations.
- Regeneration: multi-step process; cost efficiency is low; complexity is high; a good chance that it may be not scalable.

Specific recommendations and additions or deletions to the work scope

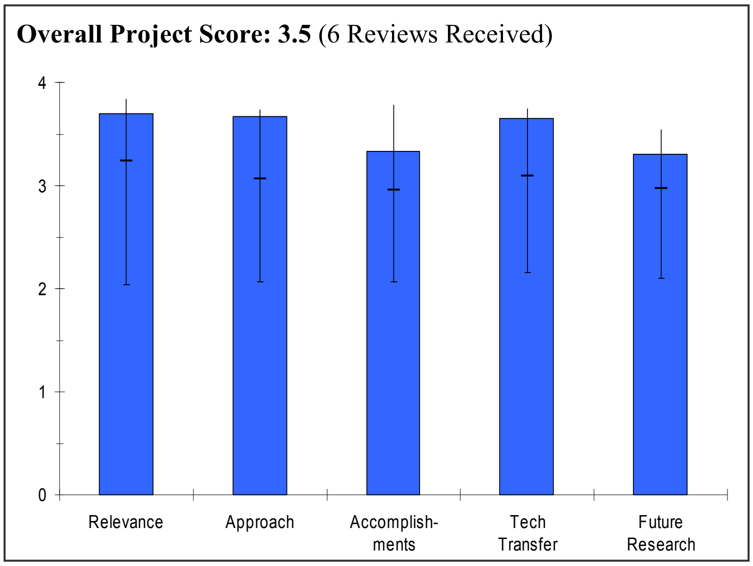
- None.
- The engineering component in the center should undertake a conceptual design of the on-board system to establish the acceptable range of materials properties and characteristics.
- Continue as planned.

Project # ST-28: PNNL Research as part of the Chemical Hydrogen CoE

Chris Aardahl; Pacific Northwest National Laboratory (PNNL)

[Member of the Chemical Hydrogen Center of Excellence]

Brief Summary of Project



This project covers the research and development (R&D) activities being conducted by PNNL as part of the DOE Center of Excellence for Chemical Hydrogen Storage. The objectives for PNNL include identification and investigation of chemical compounds that promise to meet DOE goals for storage density (gravimetric and volumetric), hydrogen release rate, and storage system and fuel costs. The approach includes assisting in evaluation of improved regeneration strategies for sodium borohydride ($NaBH_4$), examination of other boron systems such as the ammonia boranes (AB), and discovery and development of new chemical systems beyond boron. Viable bench-scale chemistry from the center will be developed into engineered approaches and demonstrated as a viable storage system.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.7** for its relevance to DOE objectives.

- The PNNL project directly supports the goals of the President's Hydrogen Fuel Initiative.
- This project fully supports the goals and objectives of the DOE Hydrogen Program. It is extremely relevant to the other center partners and serves to keep the research of the other center partners focused on developing materials that have the proper characteristics.
- The PNNL effort is a key component in the CHCoE, and the extensive work conducted by PNNL on the ammonia borane systems contributes greatly to the success of the CoE.
- AB is a key player in the chemical hydride effort. The high potential capacities (and relatively low desorption temperatures) of this material make this a potentially viable technology. But, of course, key barriers (capacity, rate, spent fuel regeneration) need to be overcome, and this effort is focused on those issues.
- SNH_3BH_3 has potential to meet the 2010 storage targets.
- Very focused project on a specific storage material with high capacities.

Question 2: Approach to performing the research and development

This project was rated **3.7** on its approach.

- Excellent mixture of experimental and computational tools. The approach is good, and seems focused on precisely the key barriers for this technology. Would be interesting to see more on the simple analysis of the energy efficiency of the various regeneration strategies.
- The approach for hydrogen release and material regeneration is well thought-out and well-focused. The critical issues and problem areas are being addressed in a careful and thorough way by a first-rate R&D team.
- A wide range of diagnostic tools and capabilities are being used to support the synthesis, testing, and modeling activities. Detailed analysis of this kind is essential for elucidating the mechanistic details and is enabling reasonable decisions to be made concerning future work on this complex system.

- The approach is completely focused on the technical barriers in the CHCoE. The engineering studies being conducted define the physical and chemical parameters that a material must have to ensure system viability. Engineering tools are being used to help direct research activities and to identify challenges.
- Solid work being conducted in parallel with the scientific studies on use of engineering-based tools to examine processes and system requirements.
- Very good approach that is focused at addressing the key issues.
- Stability of NH_3BH_3 is being investigated.
- Initial engineering system considerations are being factored in.
- Looked at additives to enhance kinetics.
- Important work on AB stability at relatively low temperatures e.g., 60°C.
- The most critical issue is still regeneration, and this is being aggressively attacked.
- Enhanced effort this year on regeneration.
- Good use of theory to guide digestion step in regeneration of AB.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.3** based on accomplishments.

- Although some questions remain concerning the nature of hydrogen release (e.g., reasons for sluggish second hydrogen equivalent kinetics, possible improvements in release rate with different additives and scaffolds), the PNNL team has done an excellent job of understanding and describing the release process. That aspect seems to be under control.
- Decomposition condition and mechanism of AB have been clarified through this project. This is expected to accelerate designation of a hydrogen generator.
- Very good progress on capacities and kinetics.
- Very nice to see the simple analysis of volumetric capacity.
- Use of new gas burette apparatus has yielded good results aimed at understanding release stages in AB.
- Showed rapid release in AB.
- Has found that surface chemistry controls plays a role in AB desorption in scaffolds, but has not made significant progress in understanding of how scaffolds work and how other scaffold materials might work. Responded to question on this by saying work was in progress.
- The emphasis on understanding and optimizing regeneration processes is a logical next-step that is being addressed in 2007. Excellent work is being done on exploring new strategies and approaches for digestion and disproportionation of spent fuel.
- One of the digestion pathways was demonstrated, although the result may be insufficient for the expectation. Efforts to find better digestion process should be continued.
- Progress on regeneration has been a little slower, but this, of course, is the most difficult issue.
- .The engineering effort on hydrogen release from AB has studied the effect of additives on the release rate and their effect on the induction period.
- Stability of solid AB is being studied. Its stability is dependent on the source of the AB indicating that the purity of the material is important.
- Engineering studies have shown the 2015 targets are not attainable with pelleted AB. An ultra-low voidage approach or the release of more H_2 from AB greater than 2 equivalents will be needed. These are significant accomplishments this year and feed important information about materials properties that are necessary to meet the DOE targets that are system based.
- Accomplishments from the current FY are somewhat modest. Most of the ideas, and even preliminary results, were presented last year: nucleation and growth (Avrami) model, effect of additives, DADB mechanism, etc.
- Given the funding level, the results are fairly modest; the expectation for this funding level should definitely be higher.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.7** for technology transfer and collaboration.

- Well connected within the center; appropriate amount of collaboration with other efforts.
- Perhaps it's not the right place for this discussion, but it would be nice to hear more about the International Partnership for Hydrogen Economy (IPHE) project.
- Strong collaboration within PNNL and across the entire CHCoE.
- Very good integration and use of collaborations.
- Appears to be very collaborative within center.
- Good new project started with IPHE partners outside of the center.
- Good use of capabilities of resources within PNNL that are supported outside of EE program (e.g., work supported by DOE's Office of Basic Energy Sciences).
- Collaboration with other center partners is very good as more promising materials are discovered.
- Theoretical studies by other center partners are guiding the efforts by the engineering team in the development of a regeneration scheme now that some promising regeneration routes are emerging.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.3** for proposed future work.

- A logical plan is in place that builds upon the extensive body of work that already exists on this project.
- Testing/optimization of lighter-weight scaffold materials should be an important objective in 2008.
- Future research is well-targeted at the key issues.
- Identified good objectives for future work – increase capacity, increase kinetics, improve efficiency of regeneration, and new proposed regeneration scheme (1 pot).
- Future work on improving the kinetics of the second equivalent will be quite interesting.
- Understanding the reasons for the decreased rate of H_2 release for the second equivalent is important future planned work.
- Understanding the impact of light scaffolds and higher loadings on H_2 release will also be studied in 2007.
- Design of a hydrogen release system from AB is strongly related to dehydrogenation condition of AB. System image and operation condition of hydrogen generator using AB should be clarified even if the image were tentative.
- Establishment of digestion of used AB fuel should be accelerated to complete total regeneration process.
- Even more important work is planned in developing a regeneration process conceptual design in 2007.
- The focus on regeneration is crucial; it could ultimately be the show-stopper for this technology.

Strengths and weaknesses

Strengths
- The material system is a strong candidate for high-efficiency storage and off-board regeneration.
- Excellent basic science work and detailed material characterization supports the overall effort.
- The team has developed an impressive understanding of the hydrogen release process and how hydrogen liberation is facilitated by nucleation and growth processes within the material.
- High hydrogen storage capacity of NH_3BH_3.
- High release rates from the solid NH_3BH_3.
- Very focused on ammonia borane as a storage material and learning how to improve its major properties – kinetics, capacity, stability and regeneration.
- The engineering team appears to have strong capabilities to guide the materials development effort. Equally important is the interaction between the theory focused parts of the center and the engineering team.

Weaknesses
- Efficient regeneration remains a serious concern. Although this is clearly recognized by the PNNL team, it wasn't clear from the presentation if the team is converging on a workable solution.
- Difficulty of regeneration of NH_3BH_3.
- Progress has been a bit slow on the regeneration process development. As feasible chemistries are discovered, progress is expected to pick up.

Specific recommendations and additions or deletions to the work scope

- Recommend that even greater attention be paid to understanding and optimizing the regeneration processes (perhaps at the expense of the systems analysis work).
- Ensure steady feedback to the materials developers regarding materials properties that are required to ensure that a pathway to meeting the 2015 targets exists.
- Some work should be undertaken to identify impurities effects on the fuel and in the H_2 that is released from the fuel.
- None.

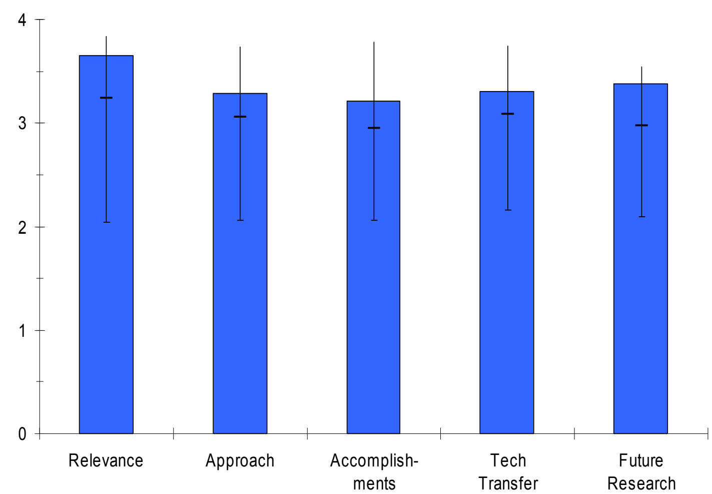
Project # ST-29: LANL Research as part of the Chemical Hydrogen CoE
Tom Baker; Los Alamos National Laboratory (LANL)

[NOTE: This review is for LANL's technical contribution to the CHCoE.]

Brief Summary of Project

The objectives of this project are to 1) provide materials chemistry support for Pennsylvania State University (PSU) work on electrochemical conversion of B-O to B-H; 2) liquefy ammonia-borane (AB) fuel and increase rate and extent of hydrogen release; 3) demonstrate chemistry and conduct engineering assessment for energy efficient AB regeneration processes; 4) continue to identify coupled chemical reactions that release hydrogen with near thermoneutrality; 5) work with International Partnership for the Hydrogen Economy partners to investigate M-B-N-H chemistry to identify potentially reversible storage systems; and 6) increase engineering efforts towards continuous processing.

Overall Project Score: 3.3 (6 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.7** for its relevance to DOE objectives.

- The ammonia borane material has potential to meet the 2010 targets.
- Project addresses relevant issues for hydrogen storage in chemical systems that have the potential for meeting the DOE storage goals.
- Work is relevant to CoE for hydrogen release and regeneration.
- Project is relevant to DOE objectives.
- This project is extremely important to the center's work on developing a process based on ammonia boranes.
- The project fully supports the DOE Hydrogen Program RD&D objectives.
- What is the role of the International Partnership for Hydrogen Economy (IPHE) project in the overall effort?

Question 2: Approach to performing the research and development

This project was rated **3.3** on its approach.

- Very effective approach utilizing members' strengths and being focused on working towards the DOE targets. I compliment the center for cutting research projects, which did not seem promising for hydrogen storage, although they were interesting research topics.
- The approach features several paths in the effort leading to a 4th quarter 2007 down selection to the most favorable routes for H_2 release and regeneration.
- A good combination of theory, experiments, and engineering.
- The liquid ammonia borane approach has engineering advantages over solid ammonia borane.
- Have integrated theory and mechanistic studies.
- Good synergy with other amino-borane projects.
- Homogeneous catalysis work for hydrogen release is preliminary and no clear strategy was described on catalyst selection with respect to organic ligand choice, or other criteria. I would be interested in the criteria driving these choices, and this may be helpful when the transition in research proceeds to heterogeneous catalysts.

- Along that same theme, I am afraid (as is the presenter) that the characteristics suitable for a successful and selective homogeneous catalyst may not be easily reproduced in a heterogeneous catalyst system.
- Have increased focus on what was the main problem with these systems, regeneration.
- Regeneration does not seem to be efficient at the current stage of development. Further progress may require new ideas/approaches.
- Sulfur-based components of the regeneration process may be a problem if hydrogen is supposed to be used in fuel cells (due to the poisoning of the metal catalyst).
- At this time there are still activities underway on numerous fronts that give the appearance of being slightly unfocused. This perception is expected to change next year following the down selection process.
- The relationship between the engineering efforts at LANL and PNNL is unclear.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.2** based on accomplishments.

- Technical accomplishments have been good the past year. Unpromising work on acid-catalyzed dehydrogenation has been stopped. Significant progress on H_2 was made. A promising S-based regeneration scheme was identified.
- Excellent experimental work overall.
- The liquid amine-borane approach may have significant potential for higher capacities.
- Very good progress with the liquid amine borane systems – this shows that LANL is addressing the wt.% and thermodynamic problems being encountered with other systems.
- The new IPHE materials are very interesting, provided that they have a reasonable reversibility.
- Information given, though limited, shows that M-B-N-H systems could be promising.
- Theory is guiding work on new catalysts to ensure that at least 2.5 H_2 equivalents are released while keeping the products soluble.
- Mechanistic studies have elucidated reaction pathways for hydrogen release from AB.
- Beginning to understand catalytic chemistry needed to obtain desired products.
- It is too soon to assess, but I suspect that catalyst cycling/deactivation could become a big issue for the hydrogen release reaction.
- Progress was slowed somewhat by the effort required to install rapid catalyst screening capability at LANL.
- Considerable work on a regeneration scheme was shown which was not evident last year.
- Potential regeneration routes have been identified.
- Have identified regeneration chemistry and scheme which should be able to exceed regeneration efficiency goal.
- Concerns are from utilization of thiols for the digestion of $B_3N_3H_6$ as well as ammonia utilization in the BX_3 reduction. NH_3 and S are poisons to fuel cells, anodes, and membrane.
- It is not quite clear how the regenerated material is going to be separated from other products and purified.
- Scalability of the proposed synthetic approaches is to be determined yet.
- I would like to have heard more about work on engineering support for ammonia borane dehydrogenation and regeneration but the presentation was too rushed to cover the amount of information in the time allotted.
- It would have been helpful to include slides providing reference to last year's reviewer comments to help judge progress this year.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.3** for technology transfer and collaboration.

- Good collaborations through the center, particularly with Northern Arizona University and University of Pennsylvania.
- International collaboration on IPHE project.
- Collaborations with other members of the Center are evident.
- Good coordination with other groups, as stated in the presentation.
- Very good apparent utilization of each member's strengths.

- Collaboration with other research institutions is excellent.
- Collaboration with materials manufacturing industry has room for improvement.
- Collaborations with the other center partners appear to be very good.
- The work at Intematix does appear to be well integrated with the efforts at LANL or with the rest of the center's efforts.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.4** for proposed future work.

- Future work appears to be building on the results of the previous year's efforts in a logical progression.
- The plan shows technical consistency and commitment to reaching DOE target.
- The major effort in 2007 should be to work through the down select process to better focus the effort on only the most promising materials.
- All of the key issues are being addressed.
- The new IPHE materials may constitute an important new avenue.
- Catalytic work for increasing H_2 release is on track.
- MBN-H systems appear to have good potential.
- I would like to see more specific plans for catalyst development on hydrogen release, especially with respect to improving selectivity to the borazine route and transforming the lessons learned from homogeneous systems to heterogeneous ones.
- Future work is formulated in very general terms.
- Regeneration of boron-based materials deserves a stronger emphasis.
- Purification of AB after the regeneration deserves more attention.
- Determining if volatile products are in the H_2 stream released from the most promising materials should be part of the work plan for 2007.

Strengths and weaknesses

Strengths
- Ammonia borane materials have potential to meet the 2010 storage targets. The liquid solvent approach may make for easier engineering of storage systems.
- Approach and methodology (such as the new multisampling GC system.)
- Consideration of energy efficiency.
- Extensive collaboration.
- Very solid experimental work.
- Good understanding of the chemistry involved and possible engineering issues.
- The team has strong capabilities and appears to interact well with other center members. There is confidence that effective catalysts for H_2 release will be developed in 2007.

Weaknesses
- Hydrogen capacity levels and hydrogen release rates for AB in solvents are lower than for solid AB.
- Efficient and low cost AB regeneration must still be established.
- Collaboration with materials manufacturing industry has room for improvement.
- I would like to have heard more about work on engineering support for ammonia borane dehydrogenation and regeneration but the presentation was too rushed to cover the amount of information in the time allotted.
- It would have been helpful to include slides providing reference to last year's reviewer comments to help judge progress this year.

Specific recommendations and additions or deletions to the work scope

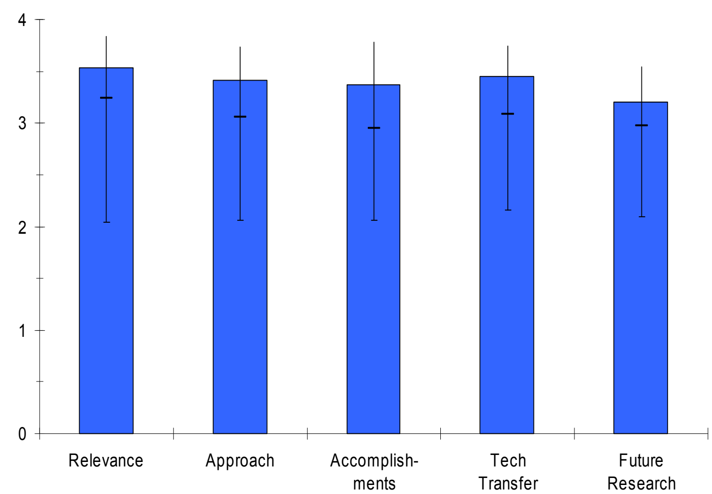
- Recommend to definitely continue this project.
- Clarify the interaction with Intematix in discovering new catalysts.
- Is the Tier 1 activity still necessary?

Project # ST-30: Main Group Element and Organic Chemistry for Hydrogen Storage and Activation
David Dixon; University of Alabama

[Member of the Chemical Hydrogen Center of Excellence]

Brief Summary of Project

Overall Project Score: 3.4 (6 Reviews Received)



The objectives of this project are to develop promising approaches to chemical hydrogen storage for future DOE targets:

- Develop new chemistries to enable DOE to meet the technical objective: "By 2010, develop and verify on-board hydrogen storage systems achieving 2 kWh/kg (6 wt.%), 1.5 kWh/L, and $4/kWh.; by 2015, 3 kWh/kg (9 wt.%), 2.7 kWh/L, and $2/kWh" by using chemical hydrogen storage systems.
- Focus on organic and main group compounds to enable new chemistries which may be able to perform better for release and regeneration by improving the energy balance. This will provide longer term alternatives.
- Develop and implement imidazolium (carbene) based H_2 activation chemistry.
- Develop and implement systems based on main group elements. Examples: nitrogen and phosphorus.
- Develop and implement cyanocarbon systems for H_2 storage.
- Provide computational chemistry support (thermodynamics, kinetics, properties prediction) to the experimental efforts of the DOE Center of Excellence for Chemical Hydrogen Storage to reduce the time to design and develop new materials that meet the DOE targets.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

- This project is extremely relevant and supports the DOE objectives through both novel computational and experimental work. Additionally, this research supports and directs the experimental research efforts within the center through computational studies and also seeks to develop and conduct its own independent experimental research.
- The broad-based first principles calculations support many aspects of the Hydrogen Initiative. At a minimum, these calculations should serve to eliminate systems that have no potential to meet DOE RD&D targets for hydrogen storage. In the best case, they may identify classes of materials that do have target-meeting potential.
- This project is making significant and important contributions to the CHCoE.
- The project, developing chemical materials and reaction process for hydrogen storage is an important part of the chemical hydrogen storage CoE, and well aligned with the DOE target.
- Synergy between theory and experiment in understanding energetics, energy barriers, and kinetics is important. The PI is to be congratulated in this regard.
- Direct relevance through experimental developments.
- Computational work supports variety of activities at the CHCoE.
- Work on cyanocarbons offers interesting new possibilities for hydrogen storage capacities in the 10 wt.% range.

Question 2: Approach to performing the research and development

This project was rated **3.4** on its approach.

- An ideal combined computational-experimental approach is used to direct the research. In particular, the computational methods are useful for determination of both thermodynamic and kinetic information (as applied to ammonia borane (AB)). These methods, however, seem to utilize gas phase data, which may not be adequate for these solid/melt reactions. Detailed comparisons/corroboration of experimental and computational data are needed to confirm reliability of models. Additional computational efforts have been devoted toward the evaluation of energetics for potential regeneration schemes for ammonia borane, a key barrier to the applicability of this storage material.
- Their independent organic-based work (cyanocarbons, carbenes, etc.) is also unique and implements both computation and experimentation toward optimization of hydrogen storage properties.
- The project provides important kinetic and reaction computational support to the CHCoE. And in addition, there is an experimental in-house effort in the development of new, novel chemical hydrogen storage materials.
- Theoretical approach to determine the accurate enthalpy of B-N-H species, reaction heats, and possible reaction paths is of great importance for exploring promising materials/reactions. It is also fine that these results have been transferred to other experimental team among the CoE.
- Develop new approaches and identify new concepts for improving release and regeneration by improving energy balance and provide theoretical support in the design of new materials.
- Experimental approach of this team does not seem to be linked closely with the theoretical part. The vision for this year is not clear. Their present target C-N-H materials contain 6-11 wt.% H, but it is not realistic that all the H can be used for the dehydrogenation/hydrogenation reaction under reasonable conditions. The expected storage capacity will not meet the 2010 target.
- State-of-the-art AB initio and DFT computational methods are employed in the theory part of the project. Claiming that calculated thermodynamic quantities are correct in the face of non-agreeing experimental data needs to be done judiciously.
- Carbene chemistry methods are used in the materials synthesis task. The focus is on control of the chemistry with respect to hydrogen storage capacity and optimization of dehydrogenation catalysts. Although not stated explicitly, the reviewer assumes that the focus is also on ambient temperature dehydrogenation processes.
- Two components in program – experimental material development and computational modeling. These appear to be quite different in scope and direction

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.4** based on accomplishments.

- A significant amount of work has been done over a short period of time. The computational research on ammonia borane (mechanistic and in particular regeneration) is very useful and seeks to overcome key barriers. The combined computation-experimental approach to material discovery of novel organic molecular and extended storage materials has also progressed with several new and different systems under investigation. Continued evaluation of these newly synthesized materials is encouraged.
- A large number of calculations on a variety of relevant systems were presented. These studies encompassed the dehydrogenation pathways for selected amino-boranes and the spent fuel regeneration energetics. This work is important because it sheds light on the energetics of one of the most promising chemical systems that has a chance of meeting H-storage goals.
- Excellent progress was reported in both computational support activities and the experimental development effort.
- Experiment: Development of oligomerization procedure for making cyanocarbons with high gravimetric density of hydrogen.
- Computational: calculation of accurate thermodynamics and bond energies of $B_xN_xH_y$ compounds; energetics of carbenes, cyanocarbons.
- Modeled regeneration schemes for AB.
- Identified higher energy requirements for release of second hydrogen equivalent.
- Good results in the theoretical part.
- The results for the experimental work are not adequate.
- There is nothing overly exciting coming from the synthesis task (yet). The possibilities and practicalities of a photo-catalyzed, H-exchange approach need to be addressed next year. It isn't obvious to the reviewer that there could be "widespread applicability."

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.5** for technology transfer and collaboration.

- Extensive and concrete transfer of knowledge, information, and expertise to a number of CHCoE members is evident. Evaluation of the dehydrogenation pathway of ammonia borane and its potential regeneration routes is particularly useful and relevant to the center activities.
- Collaboration with members of the CHCoE partners has been extensive and has made contributions to overall progress of the center.
- Theoretical results are well transferred to other teams working on amine borane among the CoE.
- The experimental collaboration is not clear.
- Close interaction of computational modeling with many Center partners.
- The computation supports multiple experimental studies by other members of center.
- Experimental program does not appear to have similar level of collaborations.
- Clearly, the computational portion of this project has broad collaboration within the CHCoE. It was not clear how connected the experimental task is to the rest of the CHCoE beyond some connection with LANL.
- The question is, who is defining the Alabama scope of work? Are the systems chosen for study at Alabama selected at the will of the Alabama PIs or are the decisions concerning research directions and specific systems for study made by the CoE in a consensus forming manner?
- Project is well coordinated with experiments.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.2** for proposed future work.

- The future experimental research activities on the carbene systems (molecular and extended) are appropriately directed and show promise.
- Theoretical approaches and transfer to collaborator are expected.
- Support center activities by providing theoretical expertise.
- Develop improved reaction mechanisms based on predictions of reaction kinetics.
- Benchmark DFT against quantum chemical approach.
- Study polymerized carbene to increase capacity.
- Also will look at derivatives of cyanocarbons.
- Experimentally – synthesize extended carbene polymers, non-metal catalysts
- Connection between theoretical and experimental teams in this project should be organized in a better way.
- The FY 2008 plans (as presented) are a logical extension of the work done to-date. However, this reviewer has a few suggestions as follows:
    - Focus on compounds that have a chance of delivering at least 10 wt.% hydrogen during system operation. The minimum compensation factor for the effect of balance of system on material capacity requirements is around 1.6. It's likely to be greater than 2.0 for most of the evolving storage materials. That means the 6 wt.% H target for 2010 requires a material that stores 9 to 12 wt.% H.
    - If you plan to pursue the photo catalytic studies, be prepared to say how a photolytic process could be applied in a practical on board system or at a regeneration station.
    - Kinetics issues are as compelling as thermodynamic issues; put more emphasis into that aspect of the FY 2008 plan.

Strengths and weaknesses

Strengths
- Multi-faceted, computational-experimental approach has been ideal for materials discovery and optimization. A great deal of high-impact research on diverse chemical hydride systems is clearly being explored.
- Activity in the theoretical part.
- Strong collaboration of the theoretical part with other members of the CHCoE.

- The P.I. interacts well with other researchers in the center providing critical understanding of mechanisms.
- The computational modeling effort is an excellent resource for the center.
- Knowledgeable PI.
- Impressive publication record.
- Strong collaborations in the computational area.
- This is an outstanding project and is an excellent example of how the center concept should work in practice.

Weaknesses
- Experimental data should be compared with computational-based calculations to ensure that these gas-phase models are indeed adequate.
- Perspective of the experimental approaches.
- Connection between the theoretical and experimental teams within this project.
- Experimental portion could benefit from additional collaborations/interactions.
- Some concern about how the scope of work at Alabama is determined. It should be done by CoE wide consensus as mentioned above.
- No noteworthy weaknesses.

Specific recommendations and additions or deletions to the work scope

- Next year, present at a bit slower pace. Some slides went by so fast that it was not possible to grasp the significance of what they reported.
- The FY 2008 plans (as presented) are a logical extension of the work done to-date. However, this reviewer has a few suggestions as follows:
  - Focus on compounds that have a chance of delivering at least 10 wt.% hydrogen during system operation. The minimum compensation factor for the effect of balance of system on material capacity requirements is around 1.6. It's likely to be greater than 2.0 for most of the evolving storage materials. That means the 6 wt.% H target for 2010 requires a material that stores 9 to 12 wt.% H.
  - If you plan to pursue the photo catalytic studies, be prepared to say how a photolytic process could be applied in a practical on board system or at a regeneration station.
  - Kinetics issues are as compelling as thermodynamic issues; put more emphasis into that aspect of the FY 2008 plan.

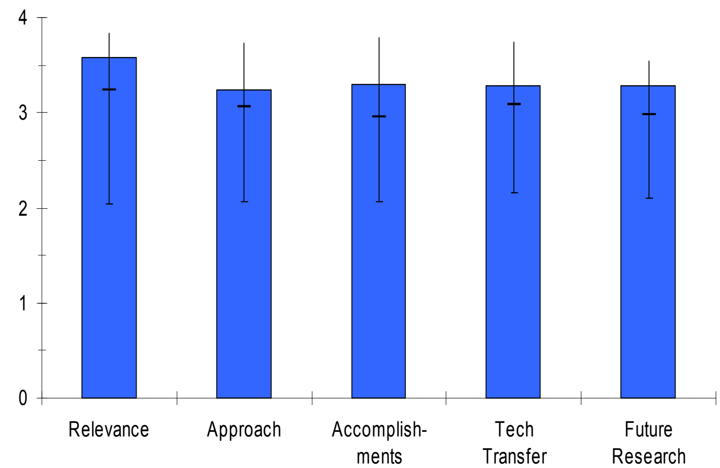
Project # ST-31: System Level Analysis of Hydrogen Storage Options
Rajesh Ahluwalia; Argonne National Laboratory (ANL)

[NOTE: This project is not part of the Centers of Excellence; it is an independent project.]

Brief Summary of Project

The objective of this project is to perform independent systems analysis for DOE on all approaches for on-board vehicular hydrogen storage technologies. Specific goals include the following:
- Model and analyze various developmental hydrogen storage systems to determine system performance (e.g. gravimetric and volumetric capacity, operability, etc.).
- Analyze hybrid systems that combine features of more than one concept.
- Develop models that can be used to "reverse-engineer" particular technologies to determine material requirements to meet DOE system targets
- Provide guidance on properties required to meet targets.
- Provide input for go/no-go decisions; and
- Identify interface issues and opportunities and data needs for technology development.

Overall Project Score: 3.3 (6 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.6** for its relevance to DOE objectives.

- This work is exactly what is needed to be able to relate performance targets to the principal contributors to reevaluate their research with respect to the overall DOE goals.
- Project results, when validated, will be key to decisions narrowing-down storage pathways.
- Storage is a major barrier to hydrogen motive applications; therefore supports development of H_2 motive market.
- Appears to be providing a good decision-making tool for DOE.
- Determination of what projects to analyze coming from DOE makes this even more relevant.

Question 2: Approach to performing the research and development

This project was rated **3.2** on its approach.

- May need to tighten some of assumptions for more realistic/ less optimistic analysis.
- Characterization of the DeH_2 [dehydrogenation hydrogen] reactor is excellent.
- Good technical work but I would like to see other reactor systems, besides trickle beds, considered.
- Generally very well designed and focused.
- Could provide more information on assumptions used – volume, etc.
- Could include sensitivity analysis of effects of changes to design – insulation thicknesses etc – to not overload the scope this could be focused on the models currently developed and should provide useful guidance to the DOE on future requirements to achieve storage targets.
- The approach is rather hard to judge form the presentation, as it would vary for each analysis since the focus for each analysis could be completely different. This is the nature of this type of work, and not a fault.
- The approach to the two analyses reported look reasonable, for the most part, although I question the importance of some of the parameters deemed important for the cryogenic pressurized tank. The hydrogen

loading for the compressed gas should not be critical here. The tank is designed to overcome this by using liquid hydrogen for long trips.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.3** based on accomplishments.

- PI accomplished an impressive array of tasks during the year under review.
- System analysis presentation is good.
- Work with LH_2 is excellent and should inform further research in LH_2 and MHCoE.
- The reverse engineering approach is good.
- Future potential is not clear because the condition of calculation is not clear.
- Very well-managed, particularly with the diverse partnership involved, and appears to be well on-target and to plan.
- Addition of some sensitivity analysis on current designs should provide sufficient depth for assessment of design parameters required in future for storage systems. This may change as other storage options become available (are developed) however.
- I've found some of the presentation graphics hard to follow, especially some of the bar charts showing results and sensitivity analyses.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.3** for technology transfer and collaboration.

- Good breadth of involvement.
- This is rather difficult to judge. Interactions are shown on the overview page, but little was said about it.
- It is assumed that at least there is tech transfer with the projects being analyzed.
- There are five publications noted.
- Some interfacing with TIAX noted in "backup slides".
- It will be critical to project success to ensure close and continuing collaboration with CoEs and other PIs.
- Further early integration will improve accuracy and relevance of analytic results.
- The demonstrated close relationship with the APCI team needs to be replicated with other CoEs.
- It is not clear how the results of this work will become part of the different CoE performance targets and goals. Will this be communicated through DOE or directly from ANL to the CoE or principal contributors?
- Should these results be used to update the Hydrogen Storage targets? For example, should the gravimetric goal also include storage efficiency and hydrogen release conversion? Presumably, these would be specific for chemical storage, metal hydrides, and carbon adsorbents.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.3** for proposed future work.

- Appears achievable and well-structured.
- This effort is externally dependent on progress elsewhere in H_2 storage. Provided there is close cooperation and adequate data exchange, it would be unfair to penalize the analysis effort based on go/no-go decisions taken in the centers.
- Care must be taken not to go too far down the analytic path on systems that are still evolving within the CoEs. To do so, risks reaching a negative analytic conclusion on a research strand that has not yet been optimized within the CoE.
- I would like to see the same systems analysis as soon as possible for metal hydrides and carbon adsorbents.
- In addition to this independent study, it would be good to have an outside firm perform a similar analysis to see how closely the results and conclusions agree.
- This looks good, especially looking at some carbon storage.

Strengths and weaknesses

Strengths

- Good program to guide principal investigators to revise their research to achieve more realistic progress toward meeting DOE goals.
- Strong leadership.
- Breadth of involvement.
- Links with other projects such as TIAX cost analysis.
- Provision of overview of design options and issues to overall DOE projects.
- Good diversity in projects analyzed.
- It combines the physical properties and the volumetric/ gravimetric system performance for the scientist.

Weaknesses

- Even given the pressure of a 20-minute presentation, it would have been beneficial to hear a broader overview of the team's analytic activities.
- It only gives a rough idea of how to improve performance, even through it is a very complicated process.
- If possible, simplify the input parameters for the easy estimation by the chemist/scientist.
- If this is the technical assessment- lack of issue raised to reach the potential, such as using the AL for the outer shell [lacking in identifying issues for reaching potential performance].
- Effect of uncertain design focus due to continuing developments.
- Some presentation materials were hard to follow.
- Perhaps there is the need for a closer look at how a project fits in to the overall HFCIT program rather than just using hard targets.
- While there may be adequate qualifications for ANL to do analyses such as these, I always question situations where National Laboratories (or other organizations for that matter) who have other funded projects within a particular program are asked to perform analyses that may involve comparisons of their own organization's projects with other projects. Independent analyses should be just that. (Note that I am not saying that there *was* anything untoward here; I seriously doubt that there would be. It is better, however, not to have even the possibility of perception.

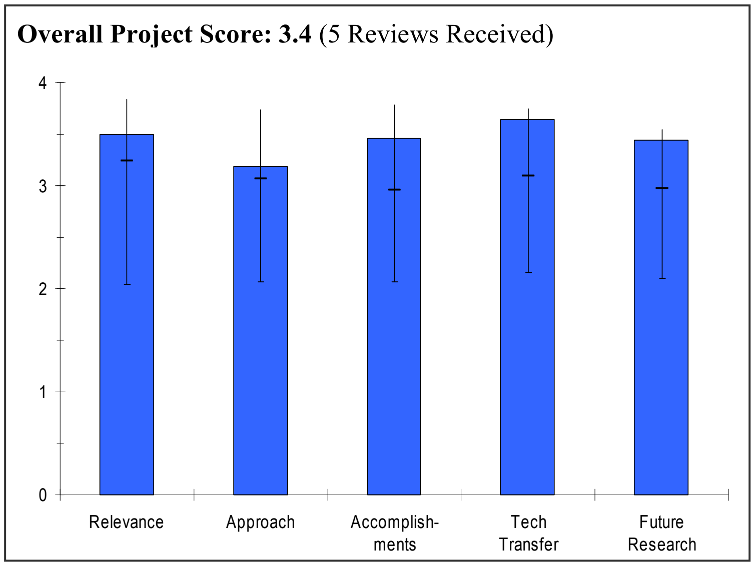
Specific recommendations and additions or deletions to the work scope

- Some of the underlying assumptions need to be crossed-checked with other stakeholders. For example, how does integrating FC operation to ATO with only 80% hydrogen consumption affect the vehicle? Would OEMs accept this? How about the transient driving cycles vs. buffer tank or battery requirements (i.e. wt.% and vol%).
- Scope appears adequate to present need.
- An extension may be required depending on the timelines of the CoEs.
- Care must be taken not to go too far down the analytic path on systems that are still evolving within the CoEs. To do so, risks reaching a negative analytic conclusion on a research strand that has not yet been optimized within the CoE.
- Addition of some sensitivity analysis on current designs should provide sufficient depth for assessment of design parameters required in future for storage systems.
- Perhaps there is the need for a closer look at how a project fits in to the overall HFCIT program rather than just using hard targets.

Project # ST-32: Analyses of Hydrogen Storage Materials and On-Board Systems
Stephen Lasher; TIAX LLC

[NOTE: This project is not part of the Centers of Excellence; it is an independent project.]

Brief Summary of Project



TIAX is evaluating the projected manufactured cost and performance of several on-board hydrogen storage options: baseline (compressed hydrogen), liquid and cryo-compressed hydrogen, reversible on-board (e.g., metal hydrides, high surface area sorbents/carbon-based materials), and regenerable off-board (e.g., chemical hydrogen storage). System-level conceptual designs, process models, activities-based cost models, and lifecycle performance/cost predictions are being developed for each system based on developers' on-going research, input from DOE and key stakeholders, in-house experience, and input from material and component experts. This is an on-going and iterative process so that DOE and its contractors can increasingly focus their efforts on the most promising technology options.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

- Cost of storage is important and the various pathways and options need both technical and economic evaluation before a valid storage option can be identified and these are key for supporting the introduction of a hydrogen motive market.
- Cost analysis of off-board and on-board hydrogen storage systems and technologies is an important part of the DOE hydrogen program.
- This effort provides valuable trend comparisons of the different types of storage and the factors that make up the total cost.
- This analysis is clearly a success requirement.

Question 2: Approach to performing the research and development

This project was rated **3.2** on its approach.

- Well structured and clear view of process.
- Excellent design, provided that models are recharged with new data from the CoEs as their efforts evolve.
- Need to cross-examine some of the assumptions to develop more realistic / less optimistic outlook.
- Needs sustained effort to integrate with H2A.
- Issues surrounding the volatility of the data and technology due to the unproven or developmental state of these has been taken in to account – reference factors compensating for safety information – good.
- Good use of sensitivity analysis.
- Flow charts very useful and presentation format showing flow of project and matrix of work undertaken and position of different types of storage very good and clear – appreciate matrix summary in presentation.
- More effort to put analyses on the same basis would be beneficial.
- Safety (sensors, etc.) systems are not included.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.5** based on accomplishments.

- Good progress on tank and on-board systems. Novel carrier work should progress in parallel with CoE effort.
- TIAX has provided relative costs of different storage systems and technologies. This information will help DOE with go/no-go decisions.
- Project appears to be very well managed.
- Revision to H2A for liquid carrier and recharge could be more fully explained.
- Although at 41% complete, very impressed with volume and quality achievements to date.
- Outstanding barrier that may be difficult to completely overcome is the current fluidity on the ultimate design of the storage devices – outstanding issues such as safety components, etc.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.6** for technology transfer and collaboration.

- TIAX is in close and frequent contact with the hydrogen storage stakeholders and energy providers to ensure appropriate technical and cost assumptions.
- Good to see that all these areas are being communicated with and are part of the partnership.
- Appears that communications are working however would have some concerns about the possibility of missing details because of the number of areas involved.
- Strong collaboration with delivery companies will be required to validate forecourt costs and options.
- Face-to-face meetings might be valuable to save time and validate approaches.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.4** for proposed future work.

- Future work is logical – finalizes the preliminary results presented at AMR 2007.
- It will remain important for the PI to stay current with improvements made outside of the CoEs that are related to storage needs, e.g., progress in cryo-tank design for medical use. Progress may come from this extremely competitive industry that could be applicable to this analysis.
- Very interested to see the output- and appears to be achievable.
- Would also like to see greater certainty in some of the cost assumptions but understand the current design situation.

Strengths and weaknesses

Strengths
- This project has provided very valuable data and is an important part of the entire storage program.
- An excellent start on a key need for the H_2 economy.
- Strong management and structured approach.
- Applicability of output.
- Focused on applicable/possible storage options.
- Clear publication of assumptions is both a requirement and a strength.

Weaknesses
- More work needs to be done to include the total costs to each possible solution in the analysis.
- Some method needs to be found to take out-of-scope cost savings into account. For example, if one were to discover a liquid storage solution, the savings from costs avoided needs to be factored in. Total cost per mile driven is the only real metric.
- Assumptions currently need to be made to allow for costs, through factorization, of some areas, such as safety, due to current uncertainty of the design requirements.

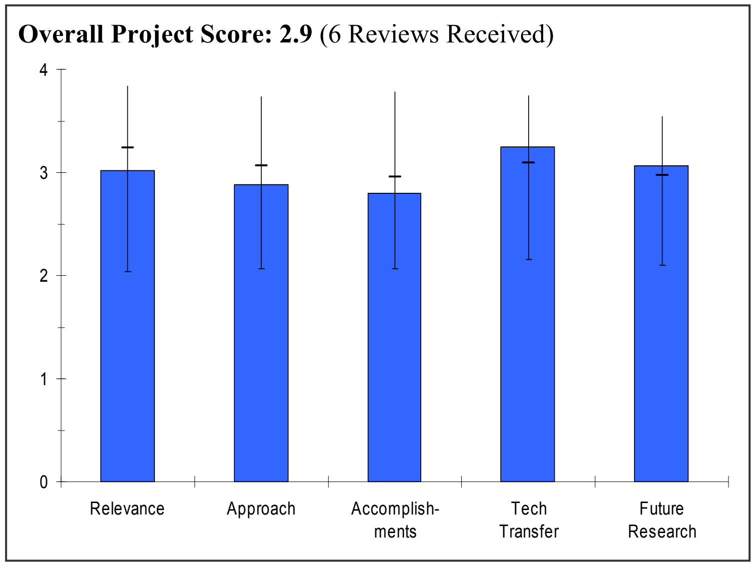
Specific recommendations and additions or deletions to the work scope

- As more cost estimates and GHG emissions data are generated, the developers need to examine the accuracy and cross-check the validity of the original assumptions (e.g., taking into account the commodity cost rise in the past three years or more accurate information on high strength carbon fibers...). On this basis, it is recommended to periodically revisit the previous estimates made in previous years with updated information.
- Substantial effort will be required to validate cost estimates associated with newly emerging chemical storage options.
- It will remain important for the PI to stay current with improvements made outside of the CoEs that are related to storage needs, e.g., progress in cryo-tank design for medical use. Progress may come from this extremely competitive industry that could be applicable to this analysis.
- Strong collaboration with delivery companies will be required to validate forecourt costs and options.
- Some method needs to be found to take out-of-scope cost savings into account. For example, if one were to discover a liquid storage solution, the savings from costs avoided needs to be factored in. Total cost per mile driven is the only real metric.

Project # ST-33: International Standardized Testing Protocols for Hydrogen Storage Materials
Karl Gross, HyEnergy

[NOTE: This project is not part of the Centers of Excellence; it is an independent project.]

Brief Summary of Project



The objective of this project is to develop and publish a reference document on best practices and limitations in measuring hydrogen storage properties of materials, including kinetics, capacity, thermodynamics and cycle life. The benefits include:
• Transferring the knowledge and experience in making critical performance measurements from experts in this field to the entire hydrogen storage research community.
• Aiding in the establishment of uniform measurement practices and presentation of uniform performance data.
• Providing a published resource to aid those just entering to this rapidly expanding field.
• Improving international communications on these issues among government, university, and industry entities and enabling the reporting of data using standardized measurement techniques.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.0** for its relevance to DOE objectives.

- This is an important project in the DOE RD&D portfolio. It will not provide the breakthrough discovery, but will assist in the establishment of uniform measurement practices and presentation of performance data. This way, it can facilitate the researcher's quest for the material that "could make the difference".
- Standardized testing procedures for candidate hydrogen storage materials would clearly be of value to the advancement of the program.
- This short project indirectly supports the DOE Multiyear RD&D plan. The resultant product will help make the absorption/desorption test procedures consistent among all DOE contractors working to meet storage materials targets.
- If the results can be quickly or fully disseminated, they would be helpful to new researchers entering the field. For senior PIs, this is frankly a limited utility, given work underway elsewhere in the Program.
- Provides support of hydrogen stgorage projects.

Question 2: Approach to performing the research and development

This project was rated **2.9** on its approach.

- Quite a straigthtforward, effective approach, tackling the main issues for conducting critical perfomance measurements - kinetics, capacity, thermodynamics and cycling life.
- The gathering of information through compiling of literature data and obtaining input from an international group of experts has been excellent. However, it is not clear how, or even if, this informantion can be assimilated into useful write-ups of generalized, "best practices" procedures.

- The approach is good. The project will review literature, presonal experience, experts' experience and advice, etc., on testing. The overall objective is to develop an open best practices document to cover definitions and procedures.
- The main aim is to reduce errors and improve measurement efficiency.
- It will help train new experts in the field. The reference document will be available to all.
- The project aims to cover the important properties: kinetics, H-capacity, thermodynamic stability, cyclic stability, activation and exit gas impurity measurement, among others.
- Success will be directly dependent on the degree to which the PI is able to secure the cooperation of CoE PIs and others who are actually working in this area.
- The objective is to generate documentation on measurement techniques applicable to hydrogen storage materials development - kinetics, capacity, thermodynamics and cycling behavior.
- Relies mainly on PI's personal experience, but also includes some input from other experts.
- Plans to use post-graduate student for some of the work.
- Documentation should be applicable to all forms of storage materials - hydrides, adsorption materials, chemical hydrides.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.8** based on accomplishments.

- Appears to be on time and on good track. Task 1 is close to completion and first deliverable is to be released soon. Data and feedback have been supplied by a number of experts in the field.
- No generalized, "best practices" procedure write-ups have been produced.
- Work has only recently begun.
- The kinetics part is about 70% done and should be delivered to DOE in draft form in two weeks.
- Work is well under way on the PCT testing.
- Some of the analysis and writing work is being done by a graduate student from UC Berkeley.
- Too early in the project to provide substantive comment.
- New project, but has initiated some documentation on one of the specific areas, namely kinetics, defined in the project.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.3** for technology transfer and collaboration.

- Experts’ involvement is already engaged in this project. Strong interface and interaction also at international level.
- The outcome of this project will be a reference document detailing best practices and limitations in measuring hydrogen storage properties of materials and will be made available to all.
- Input has been obtained from an outstanding group of international experts.
- There are many well-known and experienced collaborators contributing to the project.
- This is part of an international IEA project, including Japan and Australia.
- Outward transfer of informaton will be key to project success, but it is too early to determine if or how this is occurring.
- External collaborator list appears strong.
- Some collaborations with IEA experts, so has some international input on measurement techniques.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.1** for proposed future work.

- Near future plans are reasonable and well drawn, targeting specific barriers.
- The project though could benefit from interactions with the standardised testing facility of the SwRI which at the moment are not obvious.

- A draft of a "best practices" manual is underway. However, there appear to be no plans for the evaluation of the practical utility and subsequent refinement of the document.
- Finish survey work and report as planned.
- Appropriate start.
- Significant effort will be required to stay current with, and gain methodological agreement from PI working with new chemical storage materials.
- Proposed future work is well defined in terms of limited scope of project.

Strengths and weaknesses

Strengths
- Providing a published resource, transferring knowledge and experience particularly to new entrants in this field.
- Getting all interested parties, and particularly experts in field, involved in drawing uniform measurement practices and presentation of performance data.
- The PI is a world class expert in the measurement of the hydrogen storage properties of materials.
- A testing protocol is needed for standardization and error minimization.
- Project is being done over a very short time frame.
- It will get clear after this program is successfully completed.

Weaknesses
- Lack of plans for: 1) the assimilation of gathered information and 2) a method to obtain feedback about the practical utility of the reference document.
- Less “fascinating” topic if compared to material synthesis and development work.
- It may be prove difficult to get acceptance from the whole research community and particularly from laboratories where these measurements are routinely performed for a number of years.
- None.
- Why is data more than one year old being presented at this Review?
- At this moment it is too early to asses the result.
- It is not clear how valuable this project will be to storage program, since essentially all of the program participants are fairly knowledgeable on measurement techniques. New PIs, particularly those within centers have good resources to draw upon for help in either guiding measurements or performing them. Indeed, the examples shown in the presentation were generally drawn from results previously generated within the program.

Specific recommendations and additions or deletions to the work scope

- Liaise with the SwRI standardized testing facility.
- Could also address sample handling conditions and respective protocols integrating feedback from experts.
- Publicize final deliverables/reports in order to gain full acceptance of the quality of the reference document(s) by the research community.
- No changes recommended.

Project # STP-02: Conducting Polymers as New Materials for Hydrogen Storage

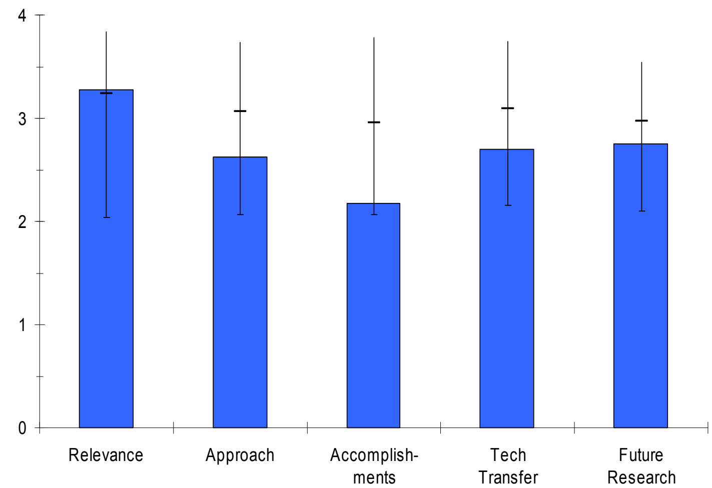
Pen-Cheng Wang, presenting; Everaldo C. Venancio, Alan MacDiarmid (Deceased), PI, University of Pennsylvania

[Member of the Hydrogen Sorption Center of Excellence]

Brief Summary of Project

The goal of this project was to identify and further develop the conducting polymer species previously reported to give ~8 wt.% hydrogen storage capacity. The project involves confirming that 8 wt.% hydrogen storage is achievable in doped forms of organic conducting polymers, polyaniline and polypyrrole; determining optimum polymer preparative methods, chemical composition, oxidation state and polymer crystallinity and morphology to give quantitative optimum conditions of hydrogen adsorption and desorption; and investigating hydrogen storage by other known types of organic conducting polymers in their semiconducting and metallic forms.

Overall Project Score: 2.6 (4 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

- Polymeric compounds represent a class of relevant materials to research for hydrogen storage. In particular, these polyaniline species are valuable to investigate as to confirm or dispute varying results which have been previously obtained.
- Generally addresses DOE goals. Success using this approach would represent a potential breakthrough in hydrogen storage.
- Project is aligned with DOE goals for hydrogen storage.
- Relevant confirmation of H_2 storage in polyaniline.
- Developing a better understanding of the nature of H_2 adsorption/desorption in polymeric materials, as well as the preparation methods that optimize H_2 uptake, is critical for developing organic-based H_2 storage materials.
- Understanding why a literature-reported result is not reproducible is valuable in helping to identify experimental shortcomings that may lead others to false conclusions.

Question 2: Approach to performing the research and development

This project was rated **2.6** on its approach.

- While the general approach to investigate the dependence of heat-treatment on the storage properties is important, it was not clear what specifically was different about the compositions (only two) that were presented. It is presumed that more than two preparation/activation methods have been attempted?
- The work in 2006 focused on identifying and understanding the properties of the polyaniline chemical sub-species undergoing reversible hydrogen sorption. The studies were conducted using combined TGA-mass spectrometry techniques. Although these methods are useful for preliminary assessments, they provide only very qualitative information concerning the amount of hydrogen release and the overall sorption behavior of the material.
- Addresses technical barriers.

- Experimental approach allows for identification of nature of the polyaniline used in the adsorption/desorption studies.
- Approach appears adequate but not comprehensive.
- Use of spectroscopic techniques to characterize the polymer systems should be incorporated into approach. It appears that techniques such as UV-VIS, SEM, NMR were used in previous years. Why were they not included in current approach?

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.2** based on accomplishments.

- In general, there seemed to be a limited variety of samples made and testing done. Additionally, this group seems to rely primarily on TGA measurements for hydrogen desorption data. Given, the resources of the sorption CoE, they should also utilize other techniques (i.e. PCT, NMR, IR, etc.) data to fully characterize samples.
- It was shown that a specific form of polyaniline (PANI-a-II) could store up to 2.8% hydrogen. The researchers were unable to replicate the higher capacity result (~6%) reported earlier by other workers. Only very qualitative information was available concerning the amount of hydrogen released upon heating. This made it difficult to evaluate the results in a meaningful way.
- Demonstrated H_2 adsorption of up to 2.8 wt.% on polyaniline.
- Demonstrated effect of thermal treatment on H_2 adsorption in polyaniline.
- Identified potentially critical issues that may invalidate previous studies reporting high H_2 adsorption on polyaniline.
- Minimal results, appears that work at Penn may have suffered as a consequence of the loss of Dr. MacDiarmid.
- Did address previous reviewer's comments by providing TGA and H_2 uptake measurements.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.7** for technology transfer and collaboration.

- The group seems to be leveraging some measurement techniques internal to their university as well as other institutions, however, it was not evident that a great deal of collaboration within the sorption CoE was made.
- There is a collaboration between workers at Penn, U of Houston, and U of Texas-Dallas. However, only a marginal connection with other partners in the HSCoE is evident.
- Collaborations with NREL and the University of Houston appear to be fruitful.
- The only role of collaborators at U of Texas-Dallas and U of Houston seem to be to provide results from characterization studies. Collaborators do not seem to be actively involved in the research aimed at improving the technology.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.8** for proposed future work.

- The future work is appropriate and relevant to the objectives of the project. In particular, additional characterization of the materials and hydrogen adsorption sites is important. PCT investigation would also highly supplement the TGA and TPD measurements that have been done thus far.
- Consideration of other new polymeric compounds for hydrogen storage would also be beneficial.
- Future research plans were not adequately motivated or described (i.e., What specific problem/issue is being addressed? What is the impact?).
- It is not clear whether the proposed plans will provide much meaninful insight into either the mechanism or optimization of the material for hydrogen storage applications.
- Proposed NMR and neutron diffraction studies should be quite useful in proof of adsorption- decorated polyaniline may lead to higher H_2 uptake.
- Neutron scattering measurements could provide valuable insight on H_2 adsorption sites.

- Introducing trace metals may improve H_2 uptake.
- Critical assumptions and issues should be incorporated into future research and addressed.

Strengths and weaknesses

Strengths
- Relevant work and extremely competent team.
- A novel hydrogen storage material system is being investigated by a research group that is internationally recognized in the field of conducting polymers.
- Careful sample preparation and identification.
- Team has done a good job to show that literature-reported H_2 uptake by polyaniline is probably not correct and that the maximum H_2 uptake appears to be 3 wt.%.
- Good work from previous years to improve our understanding of oxidation states of polyaniline.

Weaknesses
- The pace and degree of exploration seem limited.
- The idea and potential motivation for the project are interesting, and the work should be pursued. However, the overall project plan is very sketchy and the description of future work is unclear.
- The team should work more closely with other partners in the HSCoE to provide a more quantitative description of the amount of hydrogen absorption and release.
- Need to identify a project leader to replace Dr. MacDiarmid. This is critical if the project is to progress.
- Should consider broadening effort to investigate other conductive polymers now that literature-reported 6 wt.% H_2 loading on polyaniline does not appear to be achievable.

Specific recommendations and additions or deletions to the work scope

- Focus on quantitative measurements of hydrogen uptake/release.
- Focus on providing a more detailed description of hydrogen sorption in polyaniline and why certain sub-forms of the polymer will be more active.
- Provide a description of anticipated performance of an optimized PANI at realistic hydrogen delivery temperature in on-board fuel cell applications.
- "Go/no-go" type decision should be made on polyaniline and approach. Should approach be radically changed or redirected?

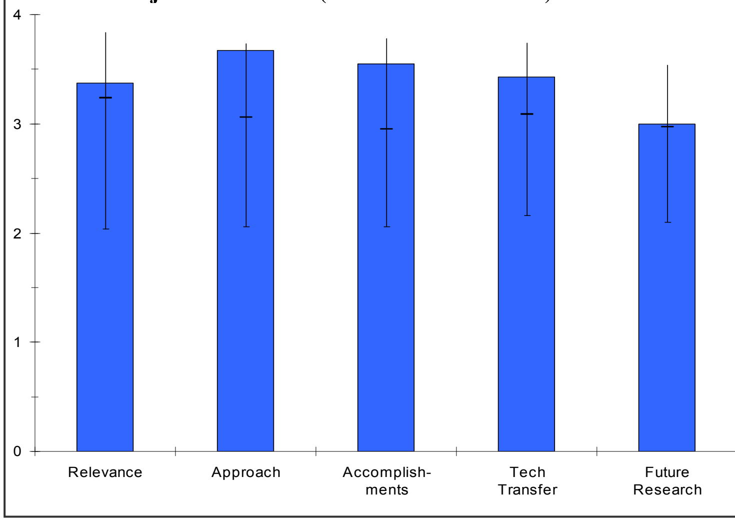
Project # STP-03: Characterization of Hydrogen Adsorption by NMR
Yue Wu (PI), Alfred Kleinhammes, Co-PI, University of North Carolina

[Member of the Hydrogen Sorption Center of Excellence]

Brief Summary of Project

The University of North Carolina is using NMR techniques to support team members of the DOE Hydrogen Sorption Center of Excellence in developing reversible materials with 7 wt.% (material) gravimetric capacity, with potential to meet DOE 2010 system-level targets. In 2007, the objectives of this project include 1) expanding the capability of the NMR adsorption system to low temperatures (77K) along with the high pressure capability (100 atm); 2) carrying out adsorption studies of single-walled carbon nanohorns; 3) understanding the effectiveness of B-doping in enhancing binding energy in graphitic carbon; and 4) analyzing the structure of B-doped carbon using NMR.

Overall Project Score: 3.4 (4 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.4** for its relevance to DOE objectives.

- Detailed and reliable characterization methods which can monitor the hydrogen adsorption/desorption process in-situ are highly valuable and critically support the sorption CoE (whose materials are often amorphous and thus more challenging to characterize). Quantification of hydrogen binding energies and hydrogen capacity are essential to this center's efforts and should be increasingly exploited. It should also be reiterated that it would be of additional value to corroborate these NMR-based measurement values with other techniques.
- Sorbents have long been one of the most promising but also the most controversial class of materials in the DOE portfolio of potential, high performance hydrogen storage materials. Resolving the long standing disputes relating to the hydrogen storage capacities and hydrogen binding energies of many members of this class of materials is a key barrier to their development.
- This work provides valuable information on amounts of hydrogen adsorbed and locations of adsorption sites. Such information is important to the development of hydrogen sorbents.
- This project proposes a powerful tool to characterize the sorption properties of hydrogen in materials.

Question 2: Approach to performing the research and development

This project was rated **3.7** on its approach.

- The techniques used appropriately focus on evaluation of hydrogen capacity and binding energy, and instrument capabilities are broadly able examine both low temperature (to LN_2) and high pressure conditions. The only apparent gap in measurement protocol is to validate NMR-based data with data from other techniques (experimentally conducted at same pressure/temperature). Although slight differences in values are expected due to sample variation and/or instrumental errors, in general, there should be correlation.
- Solid state NMR spectroscopy provides a means for the reliable determination of the hydrogen storage capacities and hydrogen binding energies associated with this class of materials.
- The development of 77K capability is very good.
- NMR capabilities are very good.

- NMR is an important tool to identify the nature of hydrogen binding in sorbents that can be used in virtually all the sorption projects.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.6** based on accomplishments.

- It is good to see increased collaboration with other projects in the sorption CoE (NREL and ORNL measurements in progress) and evaluation of a few materials under different pressure-temperature conditions. Given the demonstrated capabilities of this method, increased utilization of this tool for other systems in the HSCoE, such as the cross-linked SWNT (Rice) and Pt-spillover MOFs (Michigan), etc., is encouraged.
- Methods and hardware have been developed that allow the reliable measurement of storage capacities and binding energies associated with physisorbed and chemisorbed hydrogen. Notably, the investigators have, for the first time, determined the hydrogen capacity and binding energies of boron doped graphite through NMR techniques.
- It would have been useful to have established a calibration of the NMR hydrogen capacity measurements earlier in the project. Materials should be tested that have been corroborated by measurements at SwRI.
- Measured the binding energy of hydrogen in B doped materials (11.2 kJ/mol). Can estimate the relative contribution of adsorption sites to overall hydrogen uptake.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.4** for technology transfer and collaboration.

- This project's impact is highly dependant on the amount of collaboration that occurs with other sorption CoE projects (and other CoEs in general). Transfer of samples/data between partners seems established for NREL and ORNL and should continue to expand to others in the center.
- Good collaborations with the synthetic groups within the HSCoE. Further collaboration with groups specializing in the synthesis of MOFs is recommended.
- The project has many collaborations and the more studies that this project can perform on materials with significant potential, the better. Collaborations to run MOF materials are especially encouraged.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- Proposed plans are sound and are based on continuation of present studies (of SWNHs and B-doped graphite). As mentioned in the future work section, more focus should be placed on exploring other new sorbent materials in the center (i.e. Pt-spillover MOFs and cross-linked SWNTs). Additionally, it would also be beneficial to continue to fully evaluate each sample under a variety of conditions, both at low (~77K) and room temperature and during hydrogen desorption and adsorption.
- Future plans are too focused on materials which do not seem likely to reach the DOE targets.
- Can this project provide any useful insights into the mechanisms of hydrogen spillover at room temperature? NMR characterizations on unpromising materials should be kept to a minimum.
- Logical next steps.

Strengths and weaknesses

Strengths

- Valuable tool developed and proven for evaluation of hydrogen binding energy and capacity for physisorptive materials. This project highly compliments and supports the sorption CoE.
- NMR methods have been developed that allow the reliable determination of the hydrogen capacities and binding energies of sorbant materials.
- Technique for measuring both hydrogen content and hydrogen location in sorbent materials.
- Very important tool to advance the comprehension of the sorption process in materials.

Weaknesses

- The ultimate success and impact of this project is dependent on collaboration with its partners. Therefore, this technique should be integrated as a tool accessible to all sorption CoE partners and samples should try to be filtered through UNC as part of standard testing.
- Additional validation of NMR-based data with other techniques should be performed regularly on new samples.
- Project is concentrated on materials that are unlikely to meet the DOE targets.
- Hydrogen content measurement values need better calibration.

Specific recommendations and additions or deletions to the work scope

- Investigation of cross-linked SWNTs (Rice) and Pt-spillover MOFs (Univ. of Michigan).
- Scope of project should include the study of more advanced MOF materials.
- Studies of hydrogen spillover mechanisms should be included.
- NMR to characterize spillover (spilled-over H atoms physisorbed or chemisorbed)?

Project # STP-04: Synthesis of Small Diameter Carbon Nanotubes and Microporous Carbon Materials for Hydrogen Storage

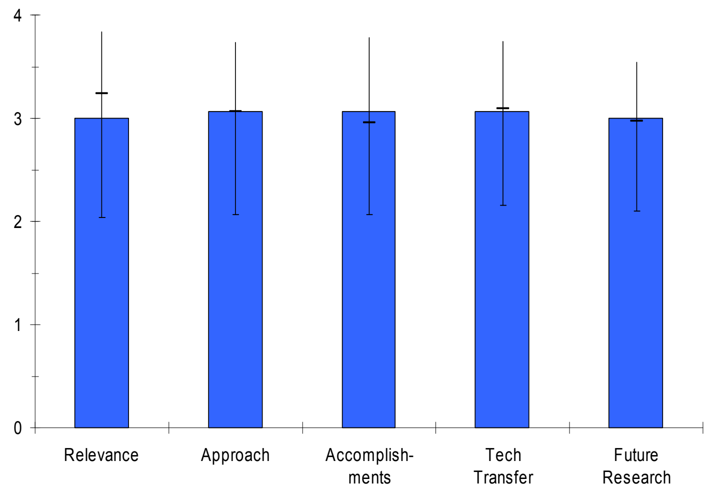
Jie Liu; Duke University

[Member of the Hydrogen Sorption Center of Excellence]

Brief Summary of Project

Goals of this project include demonstrating the storage potential of small diameter single walled carbon nanotubes and mesoporous carbon materials with metal loading to meet or exceed the DOE 2010 goal for both gravimetric and volumetric capacity. Work is underway to understand the effect of diameters of nanotubes on their hydrogen storage properties; develop a method to precisely control the diameter of the produced nanotubes; understand and demonstrate the effect of metal loading on nanotubes on the hydrogen storage properties; synthesize mesoporous carbon materials with high surface area; and study the effect of metal loading on mesoporous carbon on the hydrogen storage properties.

Overall Project Score: 3.0 (3 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.0** for its relevance to DOE objectives.

- The project serves to a certain extent the DOE objectives and supports the Hydrogen Program.
- Project on growth methods and conditions for nanotubes as well as SWNT purification is not completely novel but mostly incremental. Work on porous carbon generation from micelles precursor is a new direction and seems very promising in terms of meeting the DOE's goals regarding production scale-up and cost.
- This is one of several projects with new materials that could be important if there is a breakthrough in storage capacity.

Question 2: Approach to performing the research and development

This project was rated **3.1** on its approach.

- Following the No-Go decision on pure SWNTs, the project strategy has been redesigned, transferring existing knowledge on the pore size control of SWNT to the microporous carbon materials. Investigation of the effect of pore size and volume control on the binding energy of microporous carbons by using templates and its impact on their storage capacity.
- The porous carbon materials also offer an ideal template to study many physical phenomena including doping, spillover and pore size effect on carbon structure. The porous carbon production method is promising with regards to cost, scale-up and particle addition to the substrate. Very flexible system for control of many of the parameters.
- Research approach is narrow but focused. However, this is appropriate for a project funded at $100K.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.1** based on accomplishments.

- It is difficult to distinguish what was accomplished earlier and what are the specific achievements of the reporting period particularly with respect to the CNT diameter control. With respect to targets, an incremental improvement in specific energy has been achieved compared to 2006.
- The proposed method to generate porous carbon exists in other fields but to implement it in the context of hydrogen storage is definitely an advance that could impact the field. Work on size control for nanotubes is not completely new but completes contributions from Endo and other people working on nanotubes.
- Excellent work on material development but well short of DOE gravimetric goal. Next year, I would like to see progress on other DOE goals including volumetric capacity, adsorption, desorption, and cycle life.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.1** for technology transfer and collaboration.

- A fair degree of collaboration established within the Sorption CoE.
- Good collaboration with many group members and production of samples that can be measured by other collaborators. Expertise as a chemist is a good asset to the other team members while the PI can take advantage of other members' facilities to characterize his samples.
- Project makes good use of modeling work performed and material characterization at other institutions.
- This work is subject to crosscutting issues and may be receiving funding from other sources.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- Sensible future plans, yet a high risk area that may not deliver.
- Aggresive pursuit of the micelles based synthesis of porous carbon is the right option for future research considering the originality and promising future of the work that has been initiated.

Strengths and weaknesses

Strengths
- Long experience in SWNTs and controlling of their structure - can be the building block for the current work and could assist partners in the Sorption CoE.
- Did a lot of high quality work with very little money.
- The report is nicely presented and makes the reviewing process easy.
- The group is focusing future work on the most promising aspect of the research.
- He seems to have very strong command of his research project and where he was leading.
- Low budget cost with a possible high return.
- Good balance between fundamental and applied science.

Weaknesses
- Project presentation and clarity of ideas.
- Stability issues with materials.

Specific recommendations and additions or deletions to the work scope

- Introduce intermediate decision points/milestones for tracking down progress and fine-tuning work.
- Establish stronger collaborations and benchmark your approach against other labs' within the Sorption CoE.
- Considering the quality and quantity of the work that was done, this program should receive a funding increment.

Project # STP-06: Single Walled Carbon Nanohorns for Hydrogen Storage and Catalyst Supports
David Geohegan; Oak Ridge National Laboratory (ORNL)

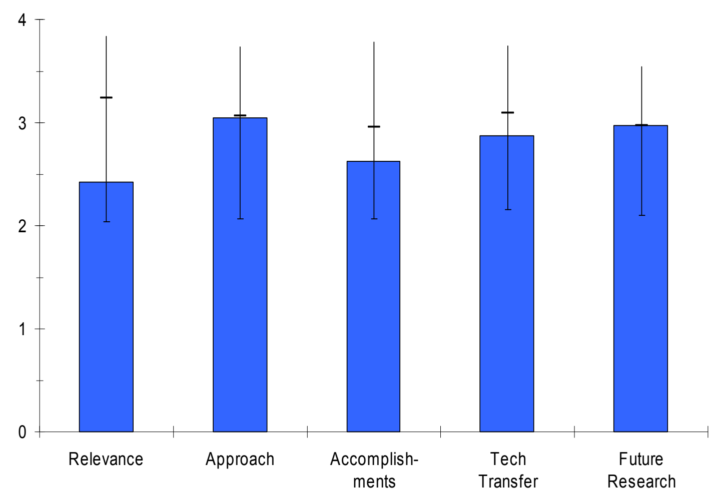
[Member of the Hydrogen Sorption Center of Excellence]

Brief Summary of Project

The overall objective of this project is to control the synthesis and processing of a novel form of carbon – single walled carbon nanohorns (SWNHs) – as a medium with tunable porosity for optimizing hydrogen storage. Specific objectives for FY 2007 include:

- Coordinate synthesis and processing treatments to tune the surface area and porosity of SWNHs, and decorate them with metal clusters;
- Vary pore size and metal decoration; work interactively with center members to clarify the dominant mechanisms of hydrogen storage in metal-decorated nanohorns to address gravimetric and volumetric DOE targets, investigate spillover, supercritical adsorption and dopant-induced charging.

Overall Project Score: 2.7 (4 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **2.4** for its relevance to DOE objectives.

- Projects explore new materials and important mechanisms that have yet to be fully understood such as the effects of spillover, dopants and supercritical absorption. Study of important hurdles that are often neglected from a systems point of view such as heat management. Emphasis on increasing enthalpy of formation and storage capacity is also important. Best results for absorption still remain very far from what is needed according to DOE and the potential to improve enough to reach targets is not clearly demonstrated. Investigation of new ideas such as introducing polarizing molecules inside nanohorns to improve sorption properties.
- The project only partially supports the DOE R&D objectives. This is an issue that should also be viewed in relevance to the recently taken No-Go decision on [pure, undoped] CNTs.
- It is difficult to understand how these molecules will be able to satisfy the DOE goals for gravimetric and volumetric capacity at non-cryogenic temperatures and at a cost that is consistent with large-scale commercialization.
- This is one of several projects with new materials that could be important if there is a breakthrough in storage capacity.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- Experiments are well designed to study the impacts of spillover, doping and structural treatments on the sorption properties of nanohorns. Interplay between theoretical modeling and experiment is apparent in the case of charge introduction within the nanohorns. It is not clear that either the nanohorns or charged structures can reach DOE's goals. This is why contributions should really focus on quantitative understanding of the described mechanisms instead of qualitative description of the improved properties, and they are planning to do this. Approach is thorough with many methods, techniques, characterization tools and collaborators. Good coupling with experimentation and theory.

- The approach seems diffuse. The investigators should focus more clearly on specific barriers and targets. 'New Directions' are proposed without clear relations to the ongoing work.
- Laser vaporization is an interesting and versatile approach for fabricating nanoscale hydrogen storage media with tunable pore size. Enhanced hydrogen adsorption on these materials requires the addition of reactive metal atoms that are incorporated in a separate processing step. Achieving hydrogen storage capacity at T > 77K is extremely challenging. These are intriguing molecules for studying basic surface reaction phenomena and for exploring the details of hydrogen sorption processes in metal-containing carbon nanostructures. However, it is not clear how adjusting the nanostructure and composition will facilitate storage at capacities and temperatures consistent with DOE goals. There is a huge gap between current observations and DOE requirements.
- I was impressed with the creative strategies and future plans. During my discussion with them, they indicated that receiving hydrogen uptake results from other institutions can sometimes be a rate limiting step for them. Thus, I support their plan to measure hydrogen uptake in house. I should have asked during my discussion with them, but I now wonder why they use only H_2PtC_{l6} to decorate with Pt. Is it possible, or have they considered, other forms of Pt with organic ligands?

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.6** based on accomplishments.

- Authors are creative in finding ways to improve sorption properties of nanostructures even if observed results still fall short of DOE's goals at this point. Progress in increasing enthalpy of formation and improving heat transfer properties show promising concepts. Given the weak storage capacity of nanohorns even with modified nanostuctures and doping, it is appropriate for them to consider investing their time on aspects of the research that have a broader reach – which they are doing through study of spillover, materials modifications, and the study of metal additions. Technical accomplishements are very substantial. Through collaboration and extensive experimental characterization, their work has advanced the field. Important issues such as heat management are investigated.
- Progress so far is modest. Work in pure nanohorns should be viewed in comparison with the recent go/no-go decision. First results from metal decorated nanohorns show decreased uptake. An accelerated rate of progress is needed.
- There is good progress on synthesizing nanostructures with tailored pore size and tunable morphology using controlled oxidative processing in CO_2. Attachment of reactive metal atoms and clusters (Pt, Pd) was successfully demonstrated and shown to promote enhanced H-adsorption. Results are consistent with a spillover mechanism. Only modest hydrogen adsorption/confinement demonstrated at room temperature. Pathway to achieving higher capacities is not clear. These are interesting materials that can be used for exploring basic surface reaction phenomena. For example, they provide a good framework for studying the details of the spillover process. However, it is highly questionable whether the adsorption mechanisms operative in these materials can result in high capacity confinement of hydrogen at non-cryogenic operating temperatures.
- Excellent work on material development but well short of DOE gravimetric goal. Next year, I would like to see progress on other DOE goals including volumetric capacity, adsorption, desorption, and cycle life.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.9** for technology transfer and collaboration.

- The team seeks the help and expertise of collaborators to perform experiments and characterize samples. The team adjusted well to last year's review regarding the lack of collaboration. More collaboration on the theoretical side leading to fundamental understanding would be of interest. No publications of past and current results are available at this point.
- Some collaboration exists but it can be significulty improved.
- Collaborations with numerous investigators within the HSCoE greatly enhance the synthetic capabilities that exist in the ORNL effort. The ORNL team has done an excellent job of providing nanostructured samples to other partners in the HSCoE.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- Orientating the project towards using polarization as a method for increasing hydrogen storage capacity is a good idea and should be pursued. A lot of their reseach for the future is aimed at understanding the fundamental physics behind the improved results that were obtained in ‘06-‘07. They are building on Iijima's work on nanohorns, opened nanohorns and decorated nanohorns. It is appropriate for them to emphasize projects that can lead to a potential breakthrough (such as understanding of spillover and supercritical absorption mechanisms).
- Plans for future research lack focus. More specific actions must be reported with regard to specific barriers (gravimetric capacity, room temp. performance…).
- Charging nanostructures is a proposed new direction that is suggested to increase the hydrogen binding energy. This concept is highly speculative and seems difficult to implement. Although it is an interesting idea, it is a serious long shot. It will be challenging to formulate a straightforward experiment that definitively demonstrates and validates this approach. There appears to be no clear pathway for increasing the storage density beyond the 0.2 - 0.8% level measured at room temperature using the spillover process.
- Future work plan looks like it will address the appropriate issues.

Strengths and weaknesses

Strengths
- The team is diverse and provides a diversified set of tools to study the proposed nanostuctures.
- The team has shown that it can build on its prior findings to advance its understanding.
- Good control over designing the nanostuctures in terms of size distrubution and morphology.
- The team proposes interesting ways to improve sorption properties through metal introduction in the nanohorns.
- Good balance of fundamental and applied research.
- The ORNL team has significant expertise and background in the synthesis and characterization of carbon nanostructures such as nanohorns using laser-based approaches. The ability to tailor the properties of the nanostructures is a big advantage over many other synthetic routes.
- Creative and novel research.

Weaknesses
- Given the resources and two years of effort, the team would be expected to have some significant publications.
- Approach and plans for future research lack focus.
- The overall work program is not coherent enough.
- The future directions should be more closely related to current activities.
- Although nanohorns provide a good platform for studying basic sorption processes in nanostructured materials, I have serious concern as to whether these materials could ever be used in a storage system that meets DOE goals for gravimetric and volumetric capacity at elevated temperatures.
- Large gap between current gravimetric results and DOE target.

Specific recommendations and additions or deletions to the work scope

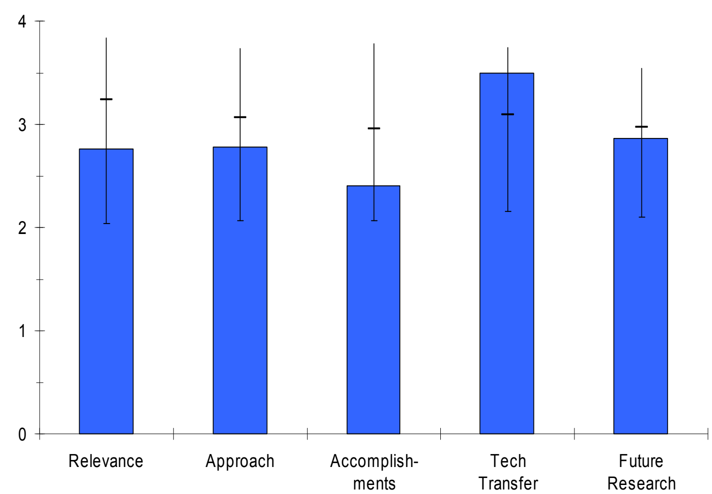
- Put emphasis on quantitative description and understanding of the spillover, effect of pore size, and supercritical absorption in the second part of this project.
- Work on explaining and predicting the enthalpy increase that is observed in metal doped structures.
- Identify what major roadblocks stand in the way of achieving high capacity storage at non-cryogenic temperatures. Provide a candid and detailed assessment of the ability of this approach to overcome those problems.

Project # STP-07: Enhanced Hydrogen Dipole Physisorption
Channing Ahn; California Institute of Technology (CalTech)

[Member of the Hydrogen Sorption Center of Excellence]

Brief Summary of Project

Overall Project Score: 2.7 (5 Reviews Received)



The goal of this CalTech project is synthesis of high surface area physisorbents (in order to achieve gravimetric densities of 7.7 wt.%) with tailored pore size (to reach volumetric densities of 58 gm/liter) and high adsorption enthalpies (ambient temperature operation). Specific objectives include:

- Further enhancement of surface area needs to be accomplished in order to improve gravimetric density (from our work, presently at 5.4 wt.% at 77K for a 2447 m^2/gm surface area activated carbon).
- Tailoring pore size needs to be addressed to maximize volumetric density (presently ~38gm/liter at 77K). Optimal pore size should be ~1.1 nm in order to maximize volumetric density.
- Sorption enthalpies beyond the 4 to 8 kJ/mole range typical of current materials needs to be increased so that sorbents can work at ambient temperatures.

Question 1: Relevance to overall DOE objectives

This project earned a score of **2.8** for its relevance to DOE objectives.

- Several project aspects and activities are in line with the program objectives. These include detailed H-uptake measurements, metal decoration of aerogels, testing of MIL materials, and thermodynamic analysis.
- Project seems mostly incremental even if results from aerogel absorption are impressive. The idea that particles can influence the sorption is a good idea but the actual results thus far are not so satisfying.
- The project includes activities that align with the programmatic vision and objectives. Nevertheless attention is needed to ensure that the relevence is kept for all its aspects.
- Developing new materials with high hydrogen capacity is in line with the DOE objectives.
- The project is concerned with carbon aerogels.

Question 2: Approach to performing the research and development

This project was rated **2.8** on its approach.

- The poster is not by itself sufficient to judge thoroughly the approach. The collaborations stated in the poster suggest good integration with other R&D. The group's work on metal decorated aerogels, MILs, and the use of its facilities and long experience on H-uptake measurements contribute to overcoming some barriers.
- Ni catalyst addition was not shown to improve sorption properties. Ideas and methodology are good. Better study of dopants on storage capacity could be obtained at room temperature where the aerogel is not already saturated because of the low temperature. The PI works on a wide range of interesting topics including aerogels, MOFs and KC24 and the comparative behaviors of these materials are potentially very interesting.
- Exploring high surface materials is a reasonable approach for finding high-capacity materials. Approaches for improving binding (sorption) energy are not presented clearly.
- So far, there has been no work at temperatures between 77K and 298K.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.4** based on accomplishments.

- The progress so far is modest. The relevant rate can be definitely improved. It seems that in many aspects, the project is simply offering high-level services to other groups (with regard to detailed uptake and thermodynamic measurements). 5.5 wt.% at 77K is claimed for a certain type of material and further improvements are expected according to the investigation.
- Interesting results on enthalpy of formation increase due to use of dopants. Good effort in order to improve the storage capacity of aerogel beyond the Chahine rule. Good ideas with the Ni nanoparticles but no results and no follow through. Good hydrogen uptake at 77K for carbon aerogels. No publications yet. Good results on carbon aerogel capacity with Baumann [LLNL].
- The progress so far is rather modest. Although the investigators expect to improve their current 5-6% , they need to better explain how they will achieve such improvement.
- High surface area materials are successfully prepared and about 5 wt.% of adsorption capacity is achieved at 77K. More detailed characterization is expected for the promising material.
- H-uptakes shown are too low to meet DOE targets. Work with Ni does not logically follow from work with pure aerogels (surface areas are different??). It is unclear how much MIL materials will be able to meet DOE targets.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.5** for technology transfer and collaboration.

- There is good collaboration and sufficient coordination with other groups (e.g., for the carbon aerogel work).
- Good collaboration with other members of the group and good exchange of ideas and materials. Many sample exchanges with other members of the group to maximize the use of the characterization tools available to the team.
- A close cooperation with other groups exists.
- Good collaboration with partners.
- Very strong collaborations with LINL and Material Institute of Lavoisier.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.9** for proposed future work.

- Plans focus on aerogels / need decoration, continuation of MILs testing. They build [on] past progress but need to address more closely how barriers will be overcome, especially at room temperature conditions.
- Incremental but good follow through with the current results. Future research is definitely building on past results and could prove interesting if successful.
- The proposed future research focuses on metal decorated carbon aerogels and MILs. There is an clear need for further elaboration on how barriers will be overcomed, especially with regard to room temperature performance.
- Some new materials such as carbon aerogel are promising. Critical vision for improving materials other than by increasing the surface area is not shown.
- No clear path forward with catalytic activation of aerogels.

Strengths and weaknesses

Strengths
- Extended facilities, long experience of the group in H-uptake measurements.
- Existing coordination/cooperation with other groups.
- The research results on aerogels are promising with the high surface area density and the above 5% storage capacity at 77K.
- The group is using collaboration well to maximize the contributions that it did with very little money.
- Adequate experience with characterization of sorbent materials.

- Systematic approach to aerogels.
- Combination of experimental techniques (PCT - microscopy).

Weaknesses
- Focus on improvements with regard to room temperature operation is needed.
- The project would benefit from additional collaboration with a theorist and a better interplay between fundamental and applied science.
- More detailed future research plans are necessary.
- The issue of performance at room temperature must be addressed in more detail.
- Low sorption enthalpy needs low temperature to keep hydrogen in the material. Vision for how to increase the sorption enthalpy is not clear.
- Future plans are not detailed enough (which catalysts, why, method by which they will be dispensed).
- Too little data were presented, or maybe, not enough experiments were carried out.

Specific recommendations and additions or deletions to the work scope

- The team is currently investigating on many fronts at the same time but results are rather incremental. But through collaboration they obtained good results for the high surface area carbon aerogel storage capacity.
- The team might benefit from chosing the direction that it considers the most promising (possibly high surface area aerogels) and pursue it more aggressively.
- The project would benefit from additional collaboration with a theorist.
- The support level should be at least 50K for one investigator.
- Surface area is apparently one of the key properties determining storage capacity. However, some other properties regarding nanostructure are possibly related to storage properties. Discussion should not be limited to surface area.
- If the project is to be a success, experimental work must be intensified (more materials, different temperatures).

Project # STP-10: Solutions for Chemical Hydrogen Storage: Hydrogenation/ Dehydrogenation of B-N Bonds
Karen Goldberg; University of Washington

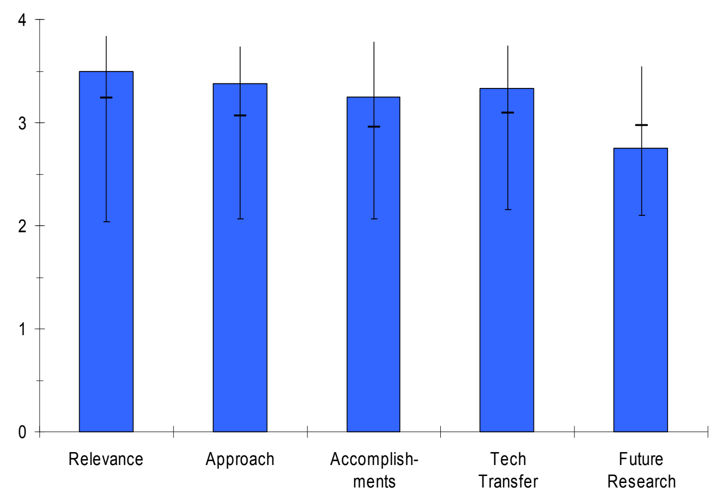
[Member of the Chemical Hydrogen Center of Excellence]

Brief Summary of Project

The objectives of this project are to:

- Identify materials/systems to meet DOE targets for gravimetric and volumetric density of H_2, focusing on amineboranes and other BN compounds with potential for high H_2 storage capacities;
- Develop catalysts to meet DOE target goals for H_2 charging/discharging rates from BN materials – thermal H_2 release from BN materials is slow and inefficient. Effective catalysts for dehydrogenation/ rehydrogenation will be needed;
- Optimize and develop cost-effective catalysts – scale of project requires inexpensive and widely available system components;
- Optimize BN materials for potential in effective regeneration processes – efficient regeneration of spent BN materials is critical.

Overall Project Score: 3.3 (4 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

- Adresses DOE goals for hydrogen storage—addresses key issues for aminoborane systems.
- The project is closely related to DOE H_2 intiatives.
- The objectives of the project are aligned with DOE RD&D ojectives.
- Finding effective and inexpensive cataysts to achieve maximum equivalence at lower temperatures with aminoborane is key to the success of this material for automotive consideration.
- Aminoborane has the potential to meet many of the DOE storage targets. However, this project does not address the very difficult cost and energy issues that are the barriers to the practical application of this material and is totally focused on the much "softer" issue of dehydrogenation kinetics.

Question 2: Approach to performing the research and development

This project was rated **3.4** on its approach.

- The approach is sharply focused on cost and reversibility.
- The PI needs to consider the reaction rate, efficiency, and selectivity when searching for a cheaper catalyst.
- BN compounds have potential as hydrogen storage materials which may meet DOE targets.
- Started with expensive materials and moving towards cheaper transition metal materials – typical approach, needs to be investigated though.
- Work to modify AB to make it reversible and slightly endothermic seems doubtful. What effect will these organic linkers, etc. have on stoarge capacity and hydrogen purity?
- The approach that has been taken is perfectly on target to overcome the barrier to achieving acceptable dehydrogenation kinetics. However, as good as this project may be, it will have little impact on overcoming the key barriers to the practical application of aminoborane.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.3** based on accomplishments.

- Demonstrated the best catalyst reported to date.
- Currently, the PI has one of the most effective catalysts for aminoborane.
- Identified catalyst for AB system that provides one equivalent of H_2 in a matter of a few minutes.
- Have identified a non-PGM catalyst which should lower cost.
- Have identified one of the problems limiting hydrogen release to first equivalent of hydrogen; however, the reaction leading to soluble product still appears to be limited to first elimination reaction (one equivalent of H_2).
- Catalysts studied appear to be limited to one equivalent of H_2 – need a system that will catalyze second elimination.
- Determined thermodynamic data for the potential of regeneration of BN compound.
- This project provides an excellent example of how fundamental studies can quickly and effectively provide guidance to the development of a practical system. Unfortunately, the value of what has been achieved can not be harnessed unless the more difficult barriers relating to re-hydrogenation can be overcome.
- Work on modifying thermodynamics of AB has just started but little details or method was offered as to how that task will be accomplished – please provide more insight.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.3** for technology transfer and collaboration.

- An excellent collaboration has been established with PNNL. Better collaboration with the investigators working on the re-hydrogenation side of the problem is critical to overall success of the effort for the practical development of this material.
- Appears to have good collaboration with other center members. All have picked up on U of Arizona's work with ammonia borane-methyl ammonia borane mixtures.
- Demonstrated close coordination with other institutions.
- Working well within the center and all appropriate partners are utilized.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.8** for proposed future work.

- Effort for the development of catalysts based on non-precious metals needs greater emphasis. Thermodynamic constraints prohibit studies of this system from having any relevance toward the elimination of the significant barriers.
- Catalyst development work attempting to build on knowledge gained from precious metal catalyst.
- Some modeling work may be beneficial.
- Plans are built on past progress and focused on overcoming the barriers.
- The catalyst development for the dehydrogenation of liquid "sovent-free" BN system is critical.
- Continue work on cheaper catalysts – crucial.
- Continue work on reducing exothermic thermodynamics of system – although success seems unlikely, it's worth a shot. This center has surprised us pleasantly before.

Strengths and weaknesses

Strengths
- The PIs are world class experts in the study of organometallic mechanisms and homogeneous catalysis. They have demonstrated the ability to quickly utilize the findings of their fundamental studies of a catalytic system to the development of a system showing significantly improved practical performance.
- Have obtained very good kinetics for the release of the first equivalent of hydrogen.
- The project has a well defined and focused research approach.

- The outcomes can be used for both on-board and off-board purposes.
- Great catalysts.
- Good center support.

Weaknesses
- Thermodynamic constraints prohibit utilization of the catalytic system to the key problem of re-hydrogenation.
- Catalysts used appear to only affect first elimination reaction.
- The PIs need to lay out a strategy to balance the cost, efficiency, and selectivity issues in developing the alternative catalyst.
- Unclear plan for reducing thermodynamics of system.

Specific recommendations and additions or deletions to the work scope

- Some modeling work may help guide catalyst search.
- Please provide plans for reducing the thermodynmacs of the system.

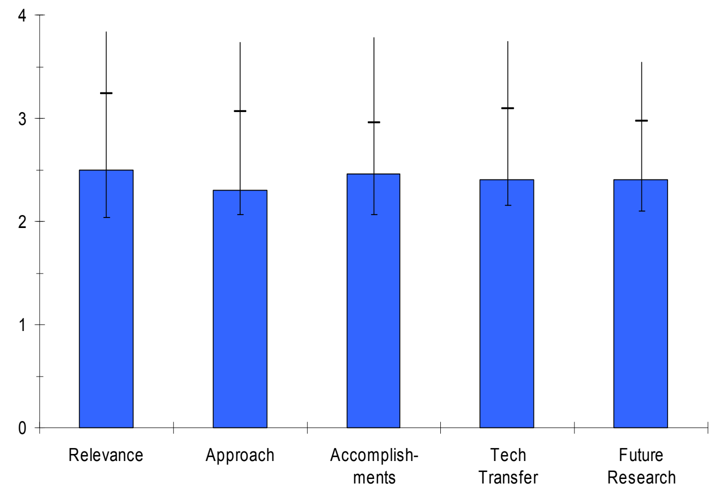
Project # STP-11: Chemical Hydrogen Storage Using Polyhedral Borane Anion Salts
Fred Hawthorne; University of Missouri

[Member of the Chemical Hydrogen Center of Excellence]

Brief Summary of Project

The objectives of this project are to:
- Develop heterogeneous catalysts for the controlled release of hydrogen from the hydrolysis of salts of $B_{12}H_{12}^{2-}$, $B_{10}H_{10}^{2-}$ and $B_{11}H_{14}^{-}$ ions.
- Determine the kinetics and mechanisms of these catalyzed polyhedral borane anion hydrolysis reactions to provide design data for large-scale hydrogen storage devices.
- Optimize existing processes for the conversion of diverse BH sources to $B_{12}H_{12}^{2-}$ and $B_{10}H_{10}^{2-}$ salts for direct use in hydrogen storage without extensive purification.
- Develop BO to BH regeneration process.

Overall Project Score: 2.4 (5 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **2.5** for its relevance to DOE objectives.

- Mixtures of polyhedral borane anions and $NaBH_4$ have the potential to meet many of the DOE storage targets. However, this project does little to address the very difficult cost and energy issues that are the barriers to the practical application of this material. It is instead focused on the much "softer" issue of dehydrogenation kinetics.
- The gravimetric capacities of this approach are somewhat marginal to meet the 2010 system target of 6 wt%.
- Relevant to stationary but likely not transportation, so aligned with some but not all program goals. Capacity is not too bad, but they don't know if they are on target for cost or efficiency goals.
- The stability of these types of materials is a definite plus.
- Cost of regeneration is a central issue.
- Polyhedral boranes have many of the same issues as sodium borohydride in terms of creating B-O bonds and only marginally better solubility characteristics in water.
- It seems quite likely that they will experience many of the same difficulties as $NaBH_4$ hydrolysis technologies do.
- Hydrolysis of polyhedral boranes has limited application to on-board storage.
- The main attributes of the system lie in the long term, stable storage of hydrogen.
- Good kinetics of release, but only effective catalyst is expensive (Rh).

Question 2: Approach to performing the research and development

This project was rated **2.3** on its approach.

- The approachs taken for developing cost effective catalysts that can effect acceptable dehydrogenation kinetics are on target. However, there is no clear approach to overcoming the key barrier of developing a practical method of BO to BH regeneration.
- Is 6 wt% the top end for these types of materials? Can the project identify any higher hydrogen gravimetric anions?

- A hydrolysis rate improvement program for polyhedral boranes, this is certainly crucial, but they are not investigating or aware of the energy lost in reaction, nor the energy of recycle, so the approach isnot realistic.
- Focused on kinetics of hydrogen release by hydrolysis of alkali metal boranes, such as $K_2B_{10}H_{10}$. These have limited capacity, require expensive catalyst (at this time) and require regeneration from BO to BH, the same as the $NaBH_4$ system.
- No regeneration work. Relies on CoE partners (Penn State, Rohm and Haas, Millenium Cell).

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.5** based on accomplishments.

- Excellent progress has been made in the development of rhodium-based dehydrogenation catalysts. However, little has been done toward the development of more ecomonically viable catalysts. Moreover, the value of what has been achieved can not be harnessed unless the more difficult barriers relating to re-hydrogenation can be overcome.
- Best initial catalyst was determined.
- Hydrogen generation rates were determined.
- Did a good deal of work but they still requires an Rh catalyst, which will be prohibitively expensive. Also looked at multiple boranes and looked at rate data. No real action on any of last year's inputs.
- Good kinetic results obtained with Rh catalysts, requiring about 1.8 liter reactor to supply 80 kW FC (at initial rate).
- Studied a number of other catalysts, but found all but Rh to be inactive.
- Measured capacities of various polyboranes ranging from about ~6 to ~6.5 wt%.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.4** for technology transfer and collaboration.

- Better collaboration with the investigators working on the regeneration side of the problem is critical to the practical development of this material.
- Need more interactions related to regeneration of the materials that are being produced.
- Collaborations might be useful to identify other types of higher gravimetric types of anions.
- Collaborations might be useful to identify alternative catalysts to rhodium.
- They are more dependent on partners than collaborating.
- Limited collaborations. Only with a few CoE partners that are working on regeneration of BO to BH.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.4** for proposed future work.

- Plans for the development of catalysts based on non-precious metals are on target. Unfortunately, no studies are planned that might be of value to solving the key, BO to BH recharging problem.
- Need to start addressing the regeneration issue, even if just on a collaborative basis.
- What about exploration for higher wt% materials?
- It would be desirable to try to identify a cheaper catalytst material than rhodium.
- Plans are suitable but they do not appear to understand the full picture enough to say if the work is worth pursuing.
- Future work described in the presentation appears limited to increasing the hydrogen generation rate and finding an alternative catalyst.

Strengths and weaknesses

Strengths
- The PI is a world class expert in the study of the reactions of boron hydrides.

- High stability of hydrogen storage materials.
- Liquid material morphology.
- High generation rates.
- PI has demonstrated good scientific capabilities and has made progress toward rapid hydrogen release from polyhedral boranes.

Weaknesses
- The value of this project to achieving the objectives of the program is tied to the “shaky” premise that a practical system can be found for the regeneration of BH from BO.
- Marginal wt% levels.
- High cost of catalyst.
- Regeneration issues.
- Even if the the gravimetrics are acceptible for stationary applications, the volumetrics are not because water has to be shipped.
- Limited scope.
- Effort is focused on materials that do not appear to have the relevant properties for achieving better on-board storage systems. However, they may have application to portable devices or long-term storage applications, so finding a low-cost catalyst could have some value.

Specific recommendations and additions or deletions to the work scope

- Project should include a task that explores some aspect of the BO to BH regeneration problem.
- None.
- More incorporation into other CoE activities would provide benefits to both the PI and the center.

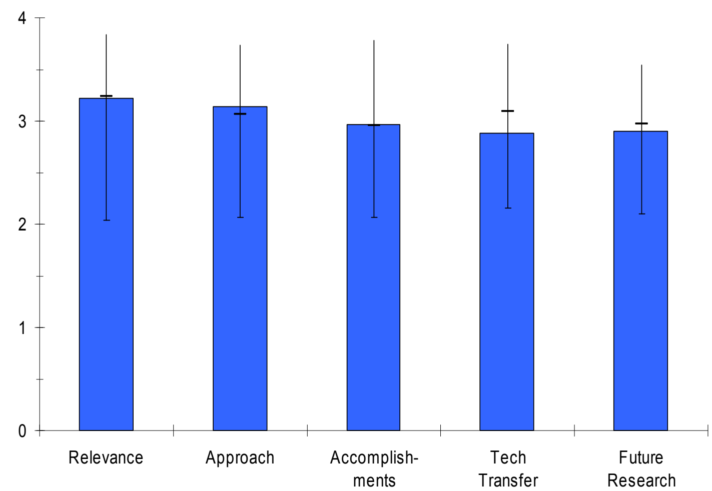
Project # STP-12: Development of Advanced Chemical Hydrogen Storage and Generation System
Oscar Moreno; Millennium Cell

[Member of the Chemical Hydrogen Center of Excellence]

Brief Summary of Project

The objectives of this project are to:
- Improve storage and release of H_2 from chemical hydrides;
- Meet the DOE 2007 target and beyond: 1.2 kWh/L (36 g H_2/L) and 1.5 kWh/kg (45 g H_2/kg);
- Leverage Millennium Cell's engineering expertise and help guide Chemical Hydrogen Storage Center research.

Overall Project Score: 3.0 (5 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.2** for its relevance to DOE objectives.

- Important systems work that directly supports DOE goals. This project offers a unique opportunity to demonstrate an entire "end-to-end" hydrogen storage system.
- The sodium borohydride system, as developed by Millenium Cell, is essentially the only chemical hydride system that has been operated on-board a vehicle. Analysis of this system and the development of engineering tools should be of value to future on-board storage systems based on chemical hydride materials.
- This project is an integral part of the DOE Hydrogen effort to develop a hydrogen storage system based on $NaBH_4$ (SBH). These are the kinds of projects that will ultimately lead to successful demonstrations of on board hydrogen storage.
- The Millennium Cell project aligns very well with the DOE RD&D objectives.
- BO to BH regeneration remains a problem on chemical hydrogen storage systems based on hydrolysis reactions for releasing stored hydrogen.
- Successful completion of the design program is critical to a positive go/no-go decision on the viability of the sodium borohydride fueling solution.

Question 2: Approach to performing the research and development

This project was rated **3.1** on its approach.

- Experimental validation of modeling results is a critical step in acquiring all of the data needed for a go/no-go evaluation in September 2007. The scope of the individual project tasks is appropriate to provide the information needed for that decision.
- The current program is focused on the engineering aspects of an on-board system based on the Millenium Cell approach. This could provide useful information for later research on chemical hydride systems.
- Good partnership with PNNL in the development of a reactor modeling tool.
- Major issues with the material system are not addressed in the current work.
- Development of engineering toolkit may be of value to other system development work.
- The overall approach is what one would expect for such a project--modeling, data gathering, experimental validations where needed, conceptual design, construction, and testing. The problem is that the project is "saddled" with a storage material (SBH) that has no real chance of meeting 2015 or even 2010 hydrogen capacity targets.

- Nonetheless, the work on this project through completion will serve as a valuable system development model for the rest of the DOE Hydrogen Program.
- The approach builds on the catalyst and reactor modeling effort over the last two years leading up to a conceptual onboard system design that is to be completed in time to allow for a preliminary cost estimate to be completed in time for the September 2007 go/no-go decision on the sodium borohydride system.
- Small-scale experiments provide data for model validation and for optimization of the reactor geometry, catalyst porosity, and pressure and temperature contol strategy.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- Good progress on development of reactor modeling—results are important to predict ultimate system performance and to provide information needed for making "mid-course" design corrections.
- Useful results obtained on defining reactor geometry and on identifying critical materials issues that could alter system performance (e.g. proper catalyst dispersion and porosity).
- Some progress made in validating reactor modeling tool. This work is continuing.
- Some effort devoted toward completing a report on all data and tools developed through this project and on pending go/no-go decision later this year.
- On-board system design improved over earlier versions. Drawing of system shows individual components and overall dimensions well, but hydrogen capacity was not stated.
- Not clear how to relate the stated hydrogen volume density value to the system depicted in the presentation. If one estimates the total volume of the individual components, the stated energy density would correspond to about a 10 kg H_2 system capacity. But if the overall dimensions are considered, the energy density is significantly lower. In any case, it isn't clear where the density numbers came from.
- It appears that enough modeling work has been done to provide a sufficient characterization of the SBH-based system for the scheduled go/no-go decision point in September 2007.
- Several key system development issues have been resolved but a few still remain unresolved.
- The key accomplishment in 2007 is the completion of the onboard hydrogen release system design. The fuel concentration was increased to 30%. The catalyst was improved to handle the more concentrated fuel and the balance of plant volume was reduced.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.9** for technology transfer and collaboration.

- Collaboration with PNNL seems to have been highly valuable to the project.
- PNNL and Rohm and Haas are the two center members with the most collaboration with Millenium Cell.
- Collaboration with PNNL is an important element of this project. Involvement with other partners in the CHS CoE seems to be limited.
- Very little collaboration, except for work with PNNL on reactor model.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.9** for proposed future work.

- The future of this project depends on the results of the go/no-go decision in September. Detailed future plans will presumably emerge from that review. Only very limited future plans given in existing presentation.
- Scope of future work limited, but probably about right for present state of the project
- The path forward hinges on the outcome of the go/no-go decision this coming September.
- Some work still needs to be completed to get fully ready for that decision, i.e., details of reactor features, balance of plant considerations, and a safety review.
- A key question for DOE is whether or not there is value in going forward with the completion of this project when the projected hydrogen system capacity performace of SBH barely meets 2007 capacity targets.

- For the remainder of FY2007 a report that compiles all the data and tools developed under this project will be generated.

Strengths and weaknesses

Strengths
- This is an important project for demonstrating and validating a fully operational hydrogen storage system.
- Success in this project could significantly impact the ultimate commercialization and utilization of hydrogen storage systems for transportation applications.
- Extensive systems experience of Millennium Cell makes that organization an ideal candidate to conduct this demonstration study.
- Strong engineering experience of Millenium Cell is being applied to increase on-board system design capabilities of the center.
- Work to date seems to have been done in a thorough and scholarly manner. The engineering looks good. The prospects for a successful demonstration of an operating SBH system seem encouraging. Unfortunately, the demo will take place no earlier than 2008 but the system will barely be able to meet 2007 metrics for overall performance. (Note: the demonstration is not until phase II of the project and will depend on the outcome of DOE’s SBH go/no-go decision)
- The preliminary design indicates that the on-board system will achieve 1.2 kWh/L and 4.5 wt.% which meets the near term DOE targets.

Weaknesses
- Demonstration system only—unlikely to meet longer-term storage objectives; degradation of catalyst properties and stability during operation can occur. This would seriously limit system performance.
- Engineering a system utilizing a material which has inherent problems with hydrogen wt.% and thermal efficiency (regeneration of the fuel) could be very difficult to optimize in an attempt to reach DOE's goals.
- The SBH demo project as a whole needs to be a bit further along to make a compelling case for being allowed to go to completion if the decision is really to be made in September of 2007.
- It is not clear that the system can meet the 2015 targets, at least a clear path to the goal is not evident.
- The current design has not yet been costed so it is uncertain if the on-board system can meet the storage system cost goal for the go/no-go decision.

Specific recommendations and additions or deletions to the work scope

- None (future work pending go/no-go decision).
- System modeling and engineering is recommended to be refocused on more promising materials.
- Devise a compelling rationale for why the project should be allowed to go to completion even though the SBH storage capacity is below target. It seems the entire Hydrogen Program will gain a great deal of valuable insight into what will be required to bring such systems to life. The list of lessons learned will be long for sure.
- Consider whether the system now on the drawing board could accommodate other types of related hydrogen storage materials.

Project # STP-13: Combinatorial Synthesis and High Throughput Screening of Effective Catalysts for Chemical Hydrides
Jonathan Melman; Intematix

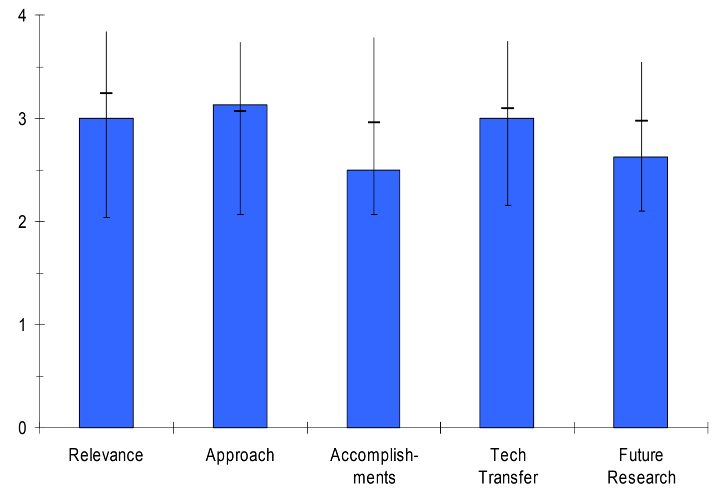
[Member of the Chemical Hydrogen Center of Excellence]

Brief Summary of Project

The objectives of this project are to discover cost-effective catalysts for release of hydrogen from chemical hydrogen storage systems to enable deployment of on-board automotive hydrogen systems; and discover cost-effective catalysts for the regeneration of spent chemical hydrogen storage materials. The specific objectives for 2007 include:

- Synthesis and screening of hydrogen-release catalyst libraries (in nano-particle and thin-film forms) to identify catalyst leads;
- Bulk tests of catalyst leads on gram scale to confirm scale-up;
- Bulk production of chosen catalyst leads for further study among center partners.

Overall Project Score: 2.8 (4 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.0** for its relevance to DOE objectives.

- This project provides important support to other partners in the CHCoE by using novel high throughput/combinatorial analysis of catalysts for the synthesis of chemical hydrogen storage materials.
- The project is very relevant to the CHCoE objectives and has the potential to be a significant contributor to the effort.

Question 2: Approach to performing the research and development

This project was rated **3.1** on its approach.

- Combinatorial screening of dehydrogenation and hydrogenation catalysts is a very effective means of discovering the most efficient catalysts in a short amount of time.
- The approach is focused on the analysis of candidate storage materials and provides important guidance and technical direction to other CoE partners.
- There does not appear to be a significant contibution to the effort from the theorists in the Center. The rationale for the selection of the catalyst library was not presented.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.5** based on accomplishments.

- Significant progress has been made in developing and applying analytical techniques to accessing potential chemical hydrogen storage materials.
- Intematix developed a few leads for suitable dehydrogenation catalysts for the center members.
- A reviewer comment from 2006 suggested that Intematix increase effort on hydrogenation catalysts; no work was reported in this area.

- It is difficult to assess progress when so few details were presented.
- There does not appear to be much progress.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- This project is basically a support activity for other partners in the CoE and, as such, they have worked closely with most of the CoE partners. Their achievements have improved the efficiency and productivity of the center as a whole.
- Intematix collaborates with PNNL, LANL, U. Penn, and Northern Arizona University on amineboranes (AB). Collaboration appears to be good.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.6** for proposed future work.

- Future plans build on the past progress and established collaborations with other center partners. Future plans also include important work on catalyst development important for regeneration of candidate hydrogen storage materials.
- Future research includes development of dehydrogenation catalysts from solution phase systems such as AB, and polyhedral boranes. The work will likely benefit from previous efforts in this area.
- Hydrogenation catalysts will also be developed but no time schedule was presented.

Strengths and weaknesses

Strengths
- This project makes important and outstanding contributions to the CHCoE.

Weaknesses
- Project scope is limited to ammonia borane systems including current and future research.
- Intematix did not provide any description of the catalyst libraries that were studied.

Specific recommendations and additions or deletions to the work scope

- Expand the scope to catalyst screening for other chemical hydrogen storage systems such as liquid hydrogen carriers.

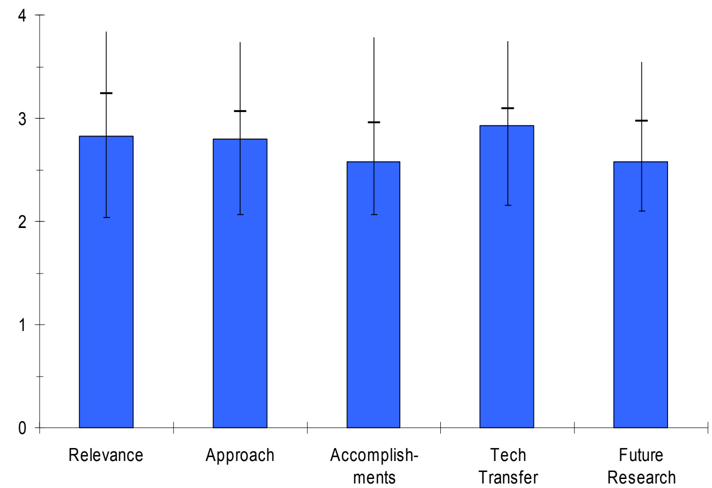
Project # STP-14: Chemical Hydrogen Storage using Ultra-High Surface Area Main Group Elements
Susan Kauzlarich; University of California-Davis

[Member of the Chemical Hydrogen Center of Excellence]

Brief Summary of Project

The goal of this project is to increase the understanding of synthetic approaches and physical properties of main group element clusters, such as Si, B, Al, and alloys thereof, BP and BN compounds and identify hydrogen storage materials with potential to meet DOE targets. Over the past year, efforts have been directed towards designing simple routes to such compounds using mild conditions and studying weight and volume capacities of the synthesized materials as well as the reversibility of hydrogen uptake. An objective is also to provide new materials, compounds, and support for chemical regeneration of amine-boranes or boron amides from B--X (X= halide or oxide) compounds.

Overall Project Score: 2.7 (4 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **2.8** for its relevance to DOE objectives.

- The work in this project is directed at the development of hydrogen storage materials and supports the DOE objectives.

Question 2: Approach to performing the research and development

This project was rated **2.8** on its approach.

- Revised plan uses the scientific capabilities of the UC Davis group to help on a specific aspect of AB regeneration. This is a nice example of effective collaboration within a center.
- Revised work plan is an improvement toward contributing to the overall CoE needs.
- Good combination of chemical synthesis and characterization of materials with spectroscopic techniques.
- Continuation of the work on high surface area materials appears to be less promising and could be redirected toward more activities in support of the CoE development efforts.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.6** based on accomplishments.

- Good progress toward synthesizing amide, hydride and formate derivatives.
- Determined quantitative yield in hydride, amide conversion to formate. Not much progress apparent on high surface area storage materials in terms of weight capacity for hydrogen.
- High surface area materials also appear to have relatively high binding energies for hydrogen, with no clear pathway indicated toward improving this parameter.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.9** for technology transfer and collaboration.

- Apparent collaboration with PNNL and LANL.
- Good collaborations and interactions within the Center.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.6** for proposed future work.

- Stated future work indicates looking at regeneration of high surface area particles. But since the materials to date do not exhibit good storage properties, it's not clear why one would spend effort on regenerating them.

Strengths and weaknesses

Strengths
- Utilization of synthetic chemical routes, preparation of nano particles.
- Excellent scientific capabilities in nanoparticle synthesis and characterization. This could lead to efficient regeneration processes for ammonia borane.

Weaknesses
- The use of non-reversible, high surface area materials for hydrogen storage appears to combine the negative properties of adsorbents (low volumetric hydrogen density), hydrides (low weight density and strong binding energy) and chemical hydrides (potentially complex off-board regeneration).

Specific recommendations and additions or deletions to the work scope

- Recommend to definitely continue this project.
- More focus on bimetallic Si compounds.
- Suggest future utilization of LANL's new GC screening system.
- The use of non-reversible, high surface area materials for hydrogen storage appears to combine the negative properties of adsorbents (low volumetric hydrogen density), hydrides (low weight density and strong binding energy) and chemical hydrides (potentially complex off-board regeneration). Perhaps this effort should be reduced further and future work should be focused more on materials development for regeneration pathways for ammonia borane, or other materials of interest to the CoE.

Project # STP-17: Hydrogen Fuel Cells and Storage Technology Project at UNLV

Clemens Heske, Balakrishnan Naduvalath (Co-PIs); Robert Perret, Project Manager, University of Nevada – Las Vegas

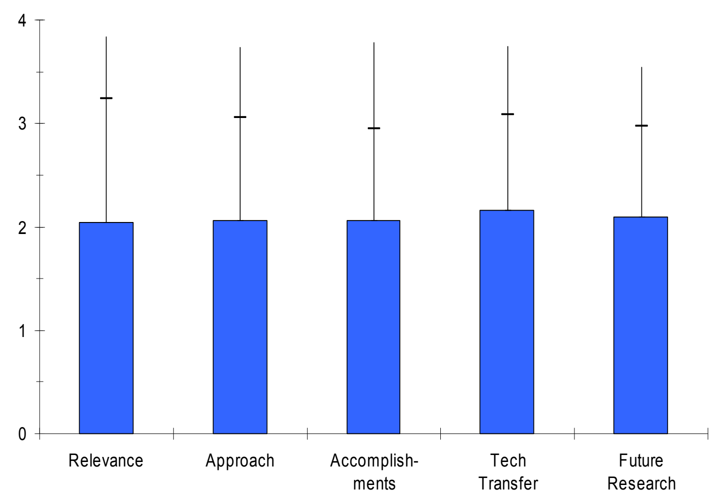
[NOTE: This project is not part of the Centers of Excellence; it is an independent project.]

Brief Summary of Project

The objective of this project is to create a framework for interdisciplinary academic research that combines theory and experiment to address specific fundamental aspects of hydrogen storage and utilization. This will be done by establishing new infrastructure (computer cluster, experimental stations, etc.) to perform integrated interdisciplinary studies on hydrogen storage, and to perform closely-coupled theoretical and experimental investigations of:

- hydrogen adsorption/desorption in various matrices to establish a solid fundamental base for optimal storage concepts;
- the electronic structure of metal hydrides, nanomaterials (C, B, N), metal adatoms, and adsorbed hydrogen molecules/atoms;
- fuel cell membranes and catalytic materials;
- Collaborate closely with external partners.

Overall Project Score: 2.1 (5 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **2.0** for its relevance to DOE objectives.

- This project seems to be aimed at storage materials that have [been] largely explored (and to some extent eliminated from further consideration) by other hydrogen storage material researchers. The possibility of new, important advancement of the storage material state-of-the-art seems highly unlikely.
- Much of the work is basic and focuses on systems that will not likely meet DOE goals. Thus far, the emphasis has been on the development of basic research capabilities that will form the foundation for future work at UNLV in the field of hydrogen storage.
- The project could support the hydrogen vision, but should align to work underway in Storage Centers of Excellence as it is working in common areas.
- A diverse project that is not fully organized toward a single track of technology. Some parts better aligned than others.

Question 2: Approach to performing the research and development

This project was rated **2.1** on its approach.

- The approach appears to be primarily a basic theoretical study complemented by experimental verification. It is not clear that new materials and their hydrogen storage capacity measurement will result from the proposed approach. This project was billed as "cross-cutting" between hydrogen storage and fuel cell enhancements, but the presenters stated that they were directed not to present their fuel cell results.
- It appears there is a lot of duplicated work which is already covered by at least one or more projects. It is not clear what strategy the PIs are developing to meet the DOE storage targets.

- Since last year, the UNLV team has done a good job of focusing its research efforts on a few specific areas. The initial effort was very delocalized. This was a serious concern that the UNLV team has obviously worked hard to address. The three tasks in the hydrogen storage area (two other fuel cell-related tasks) address useful topics. However, the work is very basic, and it is unclear whether the results of this work will have any impact on the development of a hydrogen storage material in the time frame established by the EERE program. Recommend close communication with CoE leads (esp. HSCoE-NREL in Task 1) to develop approaches and project emphasis that is complementary to on-going CoE efforts.
- Since the Carbon (Sorbent) CoE has made a "No-Go" decision with respect to pure, undoped single walled carbon nanotubes, it is not clear why work is still underway in this project.
- Some of the work is much improved from last year, the idea of probing the field on individual, identified chirality, decorated nanotubes does contribute to theory in several areas. The theory work could be useful too. Approach is not very coordinated/integrated though.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.1** based on accomplishments.

- Some progress was reported on the study of electronic structure of candidate storage materials – appliciability to DOE storage material targets and objectives is questionable although the work might contribute to basic understanding of the electronic properties of the materials under study.
- It is difficult to gauge the actual progress. The slide on technical accomplishment does not address the actual numeric results the project has achieved vs. the targets.
- The UNLV team is "coming up to speed" in areas of theory and experiment that relate to hydrogen storage. Some interesting initial progress has been made on characterizing nanostructures for enhanced hydrogen sorption and on developing new candidate metal hydride materials. It would be helpful if the results obtained in the three tasks were described in the context of previous work—i.e., What is new here? Why is it important? What are the critical issues going forward? How does it impact the selection of materials that are relevant to DOE goals? In Task 1: It is well known that Ti is a getter for oxygen, so it is not surprising that reactions with oxygen will limit hydrogen uptake in SWNTs containing Ti substituents. Also, high capacity (>9 wt.%) uptake in metal-containing organic systems is predicted. What is the predicted performance at non-cryogenic temperatures? Discussions with partners in the HSCoE could help to guide future work. In Task 2 (complex hydrides): Considerable work has been done by others. Again, a description of how the UNLV effort differs from that work and what new questions will be answered is needed. In Task 3 (PANI): Actual hydrogen uptake/release characteristics are needed (work planned). At this stage, it's not at all apparent why this approach will be superior to others employing conductive polymers.
- Lots of work going on, but not clear what has been accomplished with respect to overcoming the technical barriers of the hydrogen vision.
- Lab work has been pretty slow, especially given the large budget. Almost all results are calculations. This is the second year that we have been told they were "waiting for equipment". There is evidence that they have had a slow learning curve on using it too, and that buying equipment was put off until far later than good planning would suggest (e.g., hydrogen sorption equipment for polymers). A large bank of polymers was made and the nanotube tests are starting and the Raman mapping is starting. Several theoretical predictions were made and they constitute the bulk of the progress. More would be expected for the budget received. I am more confident than ever before though that progress in storage may emerge from this project.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.2** for technology transfer and collaboration.

- Although a number of collaborations were claimed, the nature of the collaborations and their specific contributions to the project were not clear.
- Strong collaboration exists among the members of the UNLV team (theorists and experimentalists); numerous informal external collaborations have been established. Input from other workers in the field of hydrogen storage would be useful to ensure that the topics most relevant to DOE needs are selected for future work.
- Though many collaborators identified, most work is within UNLV.
- Collaborations are present but the work still seems isolated.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.1** for proposed future work.

- Future plans appear to continue the work in progress. The project is reported to be 75% complete, thus the opportunity for additional work is limited.
- The Ti-SWNTs have been shown to be extremely good getters for oxygen. Since they can be so easily poisoned by oxygen, that greatly reduces their desirability as a candidate for future study. Work on functionalized BCN nanostructures and PANI is interesting and potentially important. Initial work should focus immediately on measurements of hydrogen uptake/release.
- Re-focus future work to support DOE technical targets complementing CoE work.
- This is much improved, but needs to move forward more toward the cutting edge of research that will get to the goals of the program.

Strengths and weaknesses

Strengths
- Enthusiastic interdisciplinary research team with broad and varied background in areas relevant to hydrogen storage research; good experimental and computational capabilities.
- The UNLV team has potential to make important contributions to the DOE program.
- Well funded.

Weaknesses
- The main focus of this work is on basic science and the researchers have only done very initial studies. It is questionable whether this approach can yield materials that are viable candidates for hydrogen storage in a time-frame that is consistent with DOE/EERE Program goals.
- $NaBH_4$ and SWNT work has been well investigated in the past, this project appears to be repeating some of that work.

Specific recommendations and additions or deletions to the work scope

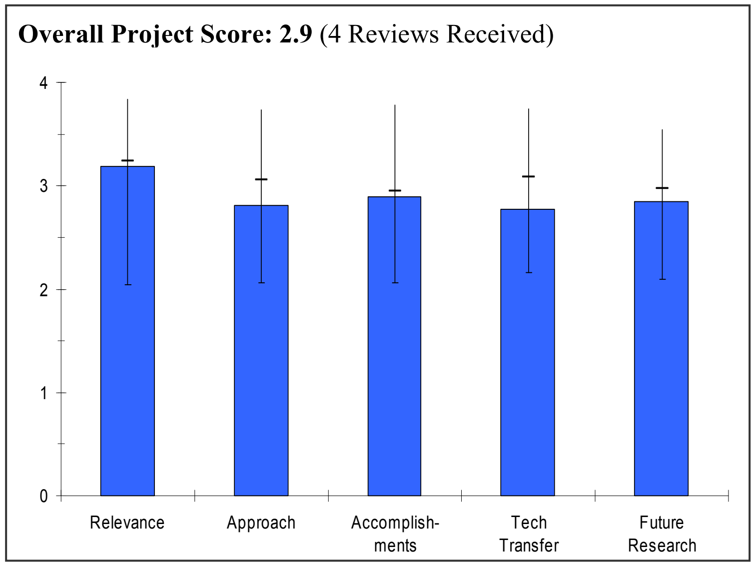
- Restructure the project to be responsive to DOE targets and goals. Focus activities on the PANI/Pd composite material and assess the potential hydrogen storage capacity.
- Candidate materials should be identified and tested for hydrogen storage capacity as soon as possible in this project. Until a good candidate material has at least been tested initially, there is concern that this project will produce an in-depth investigation of materials and processes that aren't particularly relevant to the overall DOE hydrogen storage program.
- Recommend that UNLV lead investigators engage in discussions with CoE leads concerning candidate systems and focus topics.
- Consider aligning project to a Storage CoE.

Project # STP-24: Complex Hydrides for Hydrogen Storage Studies of the $Al(BH_4)_3$ System
Gilbert Brown; Oak Ridge National Laboratory (ORNL)

[Member of the Metal Hydride Center of Excellence]

Brief Summary of Project

The objective of the project is to develop the chemistry for a hydrogen storage system based on complex hydrides, chosen from the borohydrides, amides/imides, alane, or the alanates of the light elements in the periodic table. ORNL is developing new materials and methods for synthesis of new and known materials. The ORNL goal is to employ solvent-based procedures appropriate for scale-up to production and practical application. There are two general tasks:
1. The discovery and characterization of new materials and processes.
2. The development of synthetic methods and processes in support of MHCoE collaborators.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.2** for its relevance to DOE objectives.

- The objectives of the proposal are relevant to DOE's overall objectives in pursuing the Hydrogen Fuel Initiative.
- Project fits into the President's HFI.
- Project now focuses on very high wt.% materials, clearly capable of meeting the 2010 and 2015 targets of the DOE HFCIT Multi-Year RD&D plan, if successful.
- The project is in support of DOE H_2 initiative and overall R&D objectives.
- The development of new materials and synthesis method for complex hydrides is critical to DOE targets.
- Exploring materials with a high storage capacity is oriented to the DOE objective for hydrogen storage.

Question 2: Approach to performing the research and development

This project was rated **2.8** on its approach.

- The PI is aware of the technical barriers and designed the project accordingly.
- Recent redirection of efforts has correctly moved from alanates to very high [capacity] novel borohydrides, e.g., $Al(BH_4)_3$, theoretical 16.8 wt.% H.
- Although such materials are difficult to handle and utilize in the liquid and gas states, this project's approach is of interest. Although very high risk, such activities offer potentially very high rewards.
- The work and its philosophy fit well into the MHCoE.
- The covalent borohydrides may contribute to overcoming barriers.
- The strategy of technical approach is not well defined in the poster.
- The main target material of this year is $Al(BH_4)_3$. This material is highly volatile and the decomposition reaction includes B_2H_6 emission with a high concentration. These two properties would be serious disadvantages for a storage material. However, any idea for solution is not shown clearly.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.9** based on accomplishments.

- Work has made progress against the weight barrier.
- A good understanding of the decomposition mechanism of $Al(BH_4)_3$ has been developed. The B_2H_6 intermediate poses some practical challenges vis a vis H_2 purity and practicalities.
- Up to 15 wt.% H has been measured at relatively high desorption temperature (350˚C).
- Demonstrated a substantial amount of H_2 can be obtained through the pyrolysis of $Al(BH_4)_3$.
- Achieved some fundamental understanding of the $Al(BH_4)_3$ pyrolysis mechanism.
- The PI needs to validate some experimental results.
- Characterization of $Al(BH_4)_3$ and its decomposition reaction is not accomplished enough.
- Most indications shown in the presentation (structures of $Al(BH_4)_3$ and the intermediate, reactions of B_2H_6) are not what they confirmed by themselves but what is suggested from the results already known.
- The anomalies described in accomplishments are good, which also suggests that the project needs change in direction to be fruitful.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.8** for technology transfer and collaboration.

- Good collaboration with partners.
- Good collaborations within the MHCoE are evident: GE, SNL and JPL.
- A few more collaborations might be encouraged.
- Certain coordinations exist.
- The PI needs to communicate with the theory group to obtain some theoretical understanding of the system.
- Collaboration on several characterization methods is ongoing.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.9** for proposed future work.

- Looks good to address new materials.
- Proposed continuation of efforts on the complex borohydrides and other Al complex hydrides is encouraged.
- Plans are built on past progress and may lead to some improvement.
- The PI needs to layout some strategy in determining the future research direction.
- Exploring other kinds of TM-borohydrides have been already reported by some groups. It is not clear what is the unique vision or approach of this project.

Strengths and weaknesses

Strengths
- The PI has a good group.
- Project involves unusual borohydrides with very high gravimetric capacities.
- Strong solution-based synthetic capabilities for oxygen and water sensitive materials.
- Background and experience of chemistry.

Weaknesses
- Continuation of investigation of $Al(BH_4)_3$ with problems indicated.
- Effort is very high risk. Liquid/gaseous hydrides such as these (and their intermediate borane products) will have practical handling and safety problems.
- A clear research strategy/pathway needs to be defined in this work.
- No clear perspective for exploring materials or improving the properties.

Specific recommendations and additions or deletions to the work scope

- Suggest setting a go/no-go point in the next year or so, one based on some measure of practical hope for such unusual and difficult systems.
- Highly volatile materials are not suitable for hydrogen storage because the released hydrogen should contain the vapor of the material.
- Toxicity of B_2H_6 should be addressed. This problem should be considered more seriously.

Project # STP-25: High Throughput Combinatorial Chemistry Development of Complex Hydrides
Darshan Kundaliya; Intematix

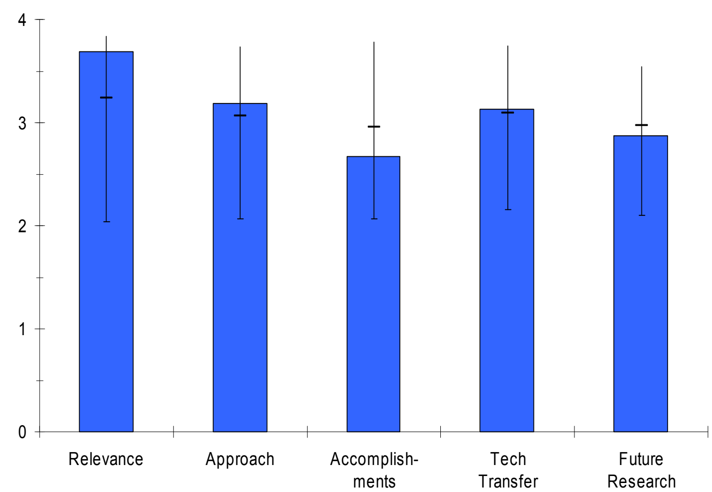
[Member of the Metal Hydride Center of Excellence]

Brief Summary of Project

The overall objectives of this project are to identify and synthesize novel metal hydride systems using high-throughput combinatorial techniques and to identify catalysts to achieve fast reaction kinetics for metal hydride systems and thus support DOE's 2010 targets for start time (4 s), flow rate (0.02 (g H_2/s)/kW) and refill time (3 min). Specific objectives for 2007 include:

- Synthesize and characterize novel complex hydride materials in thin film format;
- Continue catalyst screening on $LiBH_4$ + MgH_2 system based on leads obtained in 2006;
- Screen catalysts for various other partners/systems (GROUP A and GROUP B of MHCoE).

Overall Project Score: 3.1 (4 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.7** for its relevance to DOE objectives.

- The objectives of the proposal are relevant to DOE's overall goal in pursuing the Hydrogen Fuel Initiative.
- This project provides important support to other partners in the Metal Hydride CoE by using novel high throughput/combinatorial analysis of the synthesis of metal hydride storage materials including analysis of potential catalysts to enhance the performance of metal hydrides as storage media. In addition, the project includes independent analysis of metal hydride materials and potential catalysts to enhance material performance.
- High relevance, allows fast screening for new materials or catalysts.

Question 2: Approach to performing the research and development

This project was rated **3.2** on its approach.

- The approach is focused on the analysis of candidate storage materials and provides important guidance and technical direction to other CoE partners.
- Good approach for a rough screening of catalysts. Not so suitable for anything more subtle than H_2 is moved in and out or not. Possible false positive if the expected color change is masked.
- The project is not designed well.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.7** based on accomplishments.

- Accomplishments are fair.
- Significant progress has been made in developing and applying analytical techniques to accessing potential metal hydride storage materials.

- Suitable accomplishment pace but not clear they are really getting high throughput, not well described.
- Could be improved with help [from] analysis.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.1** for technology transfer and collaboration.

- This project has supported partners in the CoE; they have worked closely with HRL and SNL. Further collaborations are planned with other CoE partners. Their achievements have improved the efficiency and productivity of the center as a whole.
- Two patent applications have been filed.
- Reasonably well connected.
- The PI needs more collaboration.
- Collaborations need to be expanded, especially in area of data analysis.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.9** for proposed future work.

- The PI needs to address some fundamental problems related to his objectives. Using a thin film over a storage material, does not give you a good [indication] of catalysts by optical screening.
- Future plans build on the past progress and established collaborations with other center partners.
- Suitable, I hope; not too clear yet.
- Need to increase throughput.

Strengths and weaknesses

Strengths
- Handles large number of samples.
- This project makes important and outstanding contributions to the Metal Hydride CoE.
- Fast method to screen binary and ternary systems based on Mg and Li. Good experimental and theory based effort.

Weaknesses
- Basic understanding is lacking.
- More data is generated than can be analyzed. Data mining is a "choke point" that needs to be corrected. Sample geometry is cumbersome. Need to consider a single sample geometry where composition of alloys can be controlled from thin to thick prior to annealing. One sample rather than a wafer with six or more would be easier. Also, a faster screening tool such as fast IR would expedite analysis for H_2 active areas.

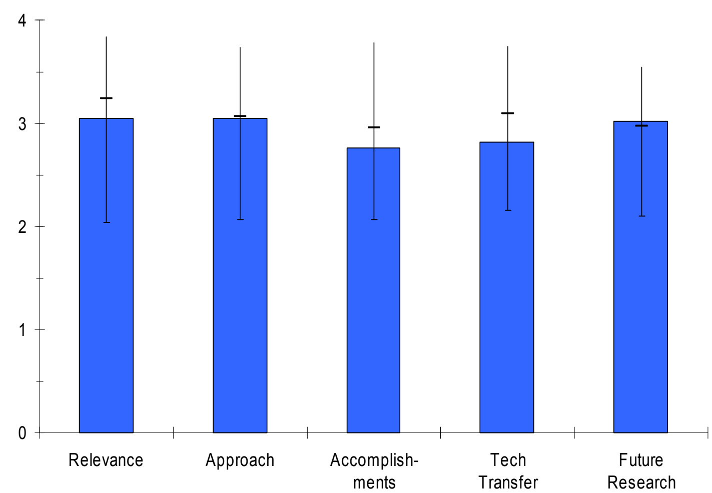
Specific recommendations and additions or deletions to the work scope

- Data mining is a "choke point" for this type of work - need to find an alternative path to increasing data mining. Consider university partnership.
- More data is generated than can be analyzed. Data mining is a "choke point" that needs to be corrected. Sample geometry is cumbersome. Need to consider a single sample geometry where composition of alloys can be controlled from thin to thick prior to annealing. One sample rather than a wafer with six or more would be easier. Also, a faster screening tool such as fast IR would expedite analysis for H_2 active areas.

Project # STP-26: Thermodynamically Tuned Nanophase Materials for Reversible Hydrogen Storage: Structure and Kinetics of Nanoparticle and Model System Materials
Bruce Clemens; Stanford University

[Member of the Metal Hydride Center of Excellence]

Overall Project Score: 2.9 (5 Reviews Received)



Brief Summary of Project

The objectives of this project include developing a fundamental understanding of metal hydride reaction kinetics. Kinetics limit practicality and reversibility of many promising metal hydride material systems. This work will focus on systems such as: .Mg, Mg_2Si, Li_4Si, $NaAlH_4$, $LiBH_4$+MgH_2. Initial work on Mg_2Si showed that kinetic issues prevented the system from achieving reversibility. Catalyst additions have shown some success in improving kinetics for some systems (ie. Ti in $NaAlH_4$), but little is known about the nature of these effects.
Little is also known about the kinetic mechanisms present in these systems, and in order to improve the kinetics for these metal hydride systems, a sound understanding must be developed.
Another project objective is to develop an understanding of metal hydride structures during phase change. Material structure can play important role in reaction kinetics, especially during solid state phase transformations such as those in metal hydride reactions. Understanding the interplay between material structure and reaction kinetics may provide insight on how to successfully engineer new materials with improved kinetics and storage properties.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.0** for its relevance to DOE objectives.

- The objectives of the proposal are relevant to DOE's overall goal in pursuing the Hydrogen Fuel Initiative.
- Aligned with DOE Hydrogen Storage Program goals.
- The project is closely related to DOE H_2 initiatives and overall R&D ojectives.
- Fundamental understanding of the reaction kinetics is critical in new material development.
- Much of the work to date, although good scientific research, has not been demonstrated to have relevance to many of the activities in the Metal Hydride CoE.
- Project is in agreement with DOE objectives.
- A basic research component is much stronger than those related to the applications.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- The project is well designed to address basic understanding of structure and kinetics of hydrogen storage material.
- Thin film approach allows for a controlled system with known structures.
- Study of kinetics in thin films should provide better understanding.
- Thin film model system and in-situ structural characterization is a good approach to get a fundamental understanding of the system.
- The approach is sharply focused on understanding the reaction kinetics.

- The Mg system should only be used as a starting point for ground work.
- The approaches should include other materials/systems.
- The argument that studying the hydriding behavior of thin films of Mg will help us understand the behavior of other hydrides prepared by bulk or nanoparticle methods is not convincing. For example, the results presented on Mg show how epitaxy can be a complicating factor in thin films compared to particles. Are the results (e.g., planar, interfacial growth rather than nucleation and growth) specific to thin films only?
- Stanford's approach is in a good agreement with the project's goals and objectives.
- Major focus: fundamental understanding of hydriding-dehydriding processes in hydrogen storage materials.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.8** based on accomplishments.

- Technical accomplishments are fair.
- This study has provided insight into mechanism, suggesting it is a moving interface growth and diffusion limited kinetics for Mg films with much faster uptake kinetics for Ti doped films.
- Cycling experiments show rapid loss of texture-leading to slower kinetics – show directions needed for further studies.
- Developed an understanding of Mg/MgH_2 phase change kinetics.
- Demonstrated using neutron reflectivity to gain insight information about kinetic mechanisms.
- Most of the results to date are on the thin film Mg system. It is understandable to begin this project by examining a single element, well studied hydride system, but it could be argued that this initial phase could have been shortened and work extended to relevant materials. It remains to be seen if new information will be obtained with this technique when applied to more complex hydride systems and studying Mg more won't contribute to answering this question.
- It is not quite clear whether data collected may be really used for material design.
- No major breakthroughs have been demonstrated so far.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.8** for technology transfer and collaboration.

- It will help to have more technical collaborations.
- Collaboration with NIST should be very valuable.
- The PI demonstrated certain coordination with other institutions.
- The PI needs to communicate with theory groups to incorporate the experimental findings into their future studies.
- Some collaborations with center partners.
- As work progresses towardsother complex systems, closer collaborations will be of value.
- Collaboration and tech transfer have room for improvement.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- Looks good.
- Planned work with quartz microbalance for thin films and nanoparticles will help bridge thin film studies to real particulates.
- Plans are built on past progress.
- The approach should be expanded to study a more promising system rather than Mg.
- Future plans are well formulated to address some of the issues discussed above – developing nanoparticle synthesis capability, direct H uptake measurement capability, and beginning a study of the Li borohydride/Mg hydride system.
- Future work looks not very convincing.

- There is a high probability that metal hydride films would quickly deteriorate during operation.
- It is not quite clear whether Mg nano-particles will "survive" handling even in a glove box.

Strengths and weaknesses

Strengths
- Good fundamental approach to understanding.
- Well defined systems to study. This leads to a better understanding of processes.
- Collaboration with NIST should allow for an even better understanding of what is occuring at the interface between the metal and metal hydride phases.
- Thin film model system and in-situ structural characterization enable a fundamental understanding of the reaction kinetics that is critical in the new material development.
- Could be a powerful tool to studying interfacial reactions in complex hydride systems.
- Much cleaner material systems can be fabricated using the techniques described here compared to other synthesis approaches. This could reveal material interactions and behavior related to the pure materials that may not be observed using other approaches.
- Good understanding of advantages and limitations of the approach used.

Weaknesses
- Limited to thin film.
- Some differences between thin films and bulk or particulates.
- The research scope needs to be expanded to include other promising materials besides Mg.
- Need to transfer the knowledge gained from this study to theory groups for their future study.
- Uncertainties remain concerning the validity of the approach as applied to more complex systems and whether or not these results will benefit other studies.
- Despite the high percent completion (40%), the project is still at a very early stage of development.
- Applicability of the results obtained is to be demonstrated.
- Unfortunately, experimental data collected for thin films may not be applicable to the bulk materials.

Specific recommendations and additions or deletions to the work scope

- Move on to other material systems.
- The research scope needs to be expanded to include other promising materials besides Mg.
- Need to transfer the knowledge gained from this study to theory groups for their future study.

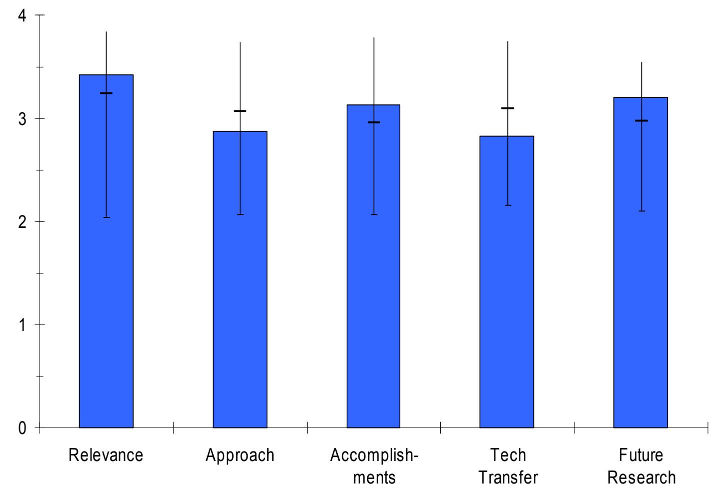
Project # STP-27: Alane Electrochemical Recharging
Ragaiy Zidan; Savannah River National Laboratory (SRNL)

[Member of the Metal Hydride Center of Excellence]

Brief Summary of Project

Alane has the potential to meet the DOE's 2010 gravimetric and volumetric system targets, but regeneration of spent material is a critical issue. The objective of this project is to directly charge and recharge alane by developing a low-cost/high-yield electrochemcial method for forming this material.

Overall Project Score: 3.1 (4 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.4** for its relevance to DOE objectives.

- Alane has the potential to meet DOE 2010 gravimetric and volumetric storage capacities. Energy efficient and cost-effective methods for recharging spent alane are critical.
- (Off-board) recharging of alane is seen as a major hurdle to use of on-board chemical hydrogen storage. This project presents an alternate to chemical recharging.
- The general technical area, on-board hydrogen storage, is very important to the DOE goals.
- Success would provide another option for recharging chemical hydrides.
- Study of a high capacity storage material is in line with the DOE target.

Question 2: Approach to performing the research and development

This project was rated **2.9** on its approach.

- The hydrogenation of Al is the most serious issue for using AlH_3. To apply an electrochemical method is one of good approaches.
- Use of non-aqueous environment to suppress oxidation of Al is an interesting approach.
- Development of high pressure, non-aqueous electrochemical cell is a move in the right direction.
- Should include characterization studies in the approach to confirm AlH_3 formation.
- Assuming a "GO" decision, will need to consider electrode durability studies.
- Significant technical risks are evident such as operating conditions and continuous operation.
- Technical hurdles are recognized and will be addressed.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.1** based on accomplishments.

- They designed the reaction cell and successfully demonstrated the formation of alane. This shows possibility of off-board regeneration.
- Good decision to abandon aqueous-based process.
- Good process on development of non-aqueous high pressure based process.
- Initial results to produce AlH_3 look encouraging. Need to begin optimizing yields and measuring rates.
- Considering the October 2006 start date, significant progress has been made.
- The technical feasibility of the approach has been demonstrated.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.8** for technology transfer and collaboration.

- Good collaboration with BNL and U of Hawaii on rehydrogenation of Al.
- Other collaboration on characterization of the product is also fine.
- Responded to FY06 reviewer's comment and increased interaction with partners BNL and U of Hawaii.
- Good interactions – use of BNL thermodynamic data to guide electrochemical cell operations.
- There is no industrial participant.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.2** for proposed future work.

- The proposed future plans are apropriate.
- Proposed future work should provide information necessary to make the go/no-go decision.
- Work to quantify yield and determine process efficiency should take top priority.
- Assuming energy efficiencies are favorable, optimizing cell performance and addressing durability issues should take second priority.
- Future work addresses questions which have arisen to date.
- Yield, efficiency, and cost need to be addressed, at least qualitatively – planned for future.
- Future work also addresses logical next steps.

Strengths and weaknesses

Strengths
- The PI has adequate experience in the field of hydrogen storage materials.
- Non-traditional approach to rehydriding metal hydride carriers.
- Development of high pressure, high temperature electrochemical cells.

Weaknesses
- Criteria for go/no-go decision are not clearly presented.
- Need to address process energy efficiency for recharging aluminum - not clear how energy cost comparing wet and electrochemical synthesis addresses this issue. A quick "high level" electrochemical energy balance - theoretical energy compared to actual energy - would be a good starting point. More detailed balances will need to consider thermal energy required to maintain cell temperature, electric power generation inefficiencies, and other process energy inputs in calculation.
- Need to develop a better approach for dealing with passive oxide layer that forms on aluminum particles.

Specific recommendations and additions or deletions to the work scope

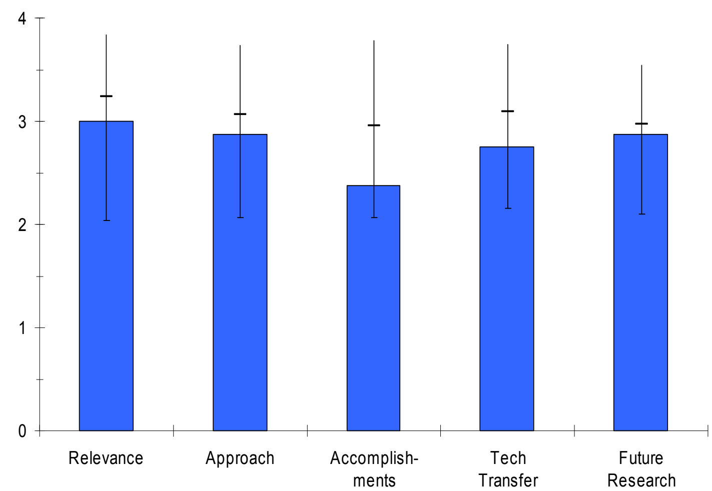
- Feasibiliy of scaling up and handling should be considered.
- Characterization of the product is recommended.
- Assuming a “GO”, electrode durability and possibility of Pt loss due to dissolution or other processes should be addressed.
- Although premature, should begin considering cycling experiments measuring rate of hydrogen discharge coupled with electrochemical hydrogen recharge to confirm the electrochemical process does not degrade hydrogen storage capacity.
- Need to address process energy efficiency for recharging aluminum - not clear how energy cost comparing wet and electrochemical synthesis addresses this issue. A quick "high level" electrochemical energy balance - theoretical energy compared to actual energy - would be a good starting point. More detailed balances will need to consider thermal energy required to maintain cell temperature, electric power generation inefficiencies, and other process energy inputs in calculation.

Project # STP-28: Synthesis of Nanophase Materials for Thermodynamically Tuned Reversible Hydrogen Storage

Channing Ahn; California Institute of Technology (CalTech)

[Member of the Metal Hydride Center of Excellence]

Overall Project Score: 2.7 (4 Reviews Received)



Brief Summary of Project

The objectives of this project are:

- To understand whether thermo-dynamically tunable reactions based on hydride destabilization, such as $Mg_2Si+2H_2 <-> 2MgH_2+Si$ that should be reversible but appear not to be, are kinetically limited;
- To address short hydrogenation times associated with refueling, that will require short solid-state and gas-solid diffusion path lengths;
- To address the problems associated with large, light-metal-hydride enthalpies (hydrogen fueling/refueling temperatures) and develop strategies to address thermodynamic issues surrounding the use of these materials through hydride destabilization. Systems of interest determined through "theoretical screening" by center partner members;
- To understand issues related to grain growth and surface/interface energies, vital in order to optimize the kinetics of hydrogenation/dehydrogenation reactions;
- To follow up on previously studied reactions with phase identification via X-ray diffraction, NMR and transmission electron microscopy.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.0** for its relevance to DOE objectives.

- Discovery of novel, high-capacity, reversible reactions is the ultimate goal of many in this field. This project is directed at this goal.
- Most of the project objectives are aligned with DOE R&D ojectives.
- Synthesis of destabilized hydride systems and analysis of reaction kinetics is critical in meeting DOE targets.
- This project is reasonably well aligned with the goals of the Metal Hydride CoE. The selection of materials is guided by computational work done in other parts of the CoE, so the outcomes are determined in part by how fruitful the recommendations turn out to be.
- The findings of this project, whether favorable or not, are of value in that they elucidate performance limiting effects the calculations don't address.

Question 2: Approach to performing the research and development

This project was rated **2.9** on its approach.

- Destabilized metal hydrides are synthesized and characterized.
- Physicochemical hydrogenation measurements are coupled with appropriate materials characterization methods to sort out the relationship between predicted behavior and experimental observations.
- Nice to see this group quickly testing theoretical predictions in the lab. Experimental efforts seem to be carefully done, reliable, and reproducible.

- Looking at systems which are irreversible (and possibly kinetically limited) may be academically interesting but information being obtained is not helping advance systems toward obtaining H_2 storage goals.
- Studying systems which will not meet cost targets.
- The "theoretical screening" approach is very efficient.
- The experimental findings do not necessarily agree with the theoretical prediction; the PIs need to address this issue in their approach.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.4** based on accomplishments.

- Tested several theoretically-predicted reactions. Unfortunately, most results were negative.
- ScH_2-$LiBH_4$ system appears to be non-reversible, products observed in NMR and X-ray do not correlate with those predicted.
- NMR studies of value in following reactions.
- First direct mechano-synthesis of $Ca(AlH_4)_2$-$LiBH_4$ system.
- Demonstrated a low reaction enthalpy system.
- Need some fundamental understanding of $Ca(AlH_4)_2$ + $2LiBH_4$ system.
- Need to validate the reaction mechanism.
- Several "theory recommended" systems were investigated.
- Experimentally determined desorption temperatures were higher than predicted. Kinetic limitations seemed to be the reason.
- Some informative materials characterization work was completed.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.8** for technology transfer and collaboration.

- Very nice to see this experimental group quickly testing theoretically predicted reactions (despite the largely negative results); would be nice for the Sorbent CoE to emulate this model.
- Collaborations not clear.
- The PI demonstrated certain coordination with other institutions.
- The PI need communicate with theory groups to incorporate some of the experimental findings into their future study.
- The project is guided in part by recommended systems for study determined in other parts of the CoE. It's good to have a few projects like this to explore the predictions of the theory component of the CoE.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.9** for proposed future work.

- Proposed future research seems like a reasonable direction, particular the aerogel work and the determination of whether this affects thermodynamics or kinetics.
- Much of the proposed future work relies on aerogel scaffolds, scaffold work has run into some problems in the chemical hydrogen storage center, decrerasing effectiveness at higher loadings.
- NMR studies could provide very useful information.
- Plans are built on past progress.
- When setting a future research direction based on some of the literature results, the PI needs to validate some of the claims first in order to efficiently direct the available resources.
- The future plans are in part a logical extension of prior work. But, there are eight or nine task areas, which seems like too many for a project of this size.
- It might be better to interact with the planning component of the Metal Hydride CoE to determine which tasks deserve the highest priority and to focus on those tasks.

Strengths and weaknesses

Strengths
- NMR studies.
- "Theoretically screened" approach is very efficient.
- Good collaboration effort with different groups.
- An enthusiastic PI and a hard working group of students.

Weaknesses
- Have been investigating systems which are not likely to meet targets (cost, reversibility).
- The experimental finding that is different from theory prediction needs to filter through to the theory group and be incorporated into future theory prediction.
- If this project is going to continue to be guided by the recommendations/results from other parts of the CoE, the results of their work may continue to be uninspiring albiet useful and interesting.

Specific recommendations and additions or deletions to the work scope

- Refinement of the future plans is recommended with input from the CoE.
- The future plans are in part a logical extension of prior work. But, there are eight or nine task areas, which seems like too many for a project of this size.
- It might be better to interact with the planning component of the Metal Hydride CoE to determine which tasks deserve the highest priority and to focus on those tasks.

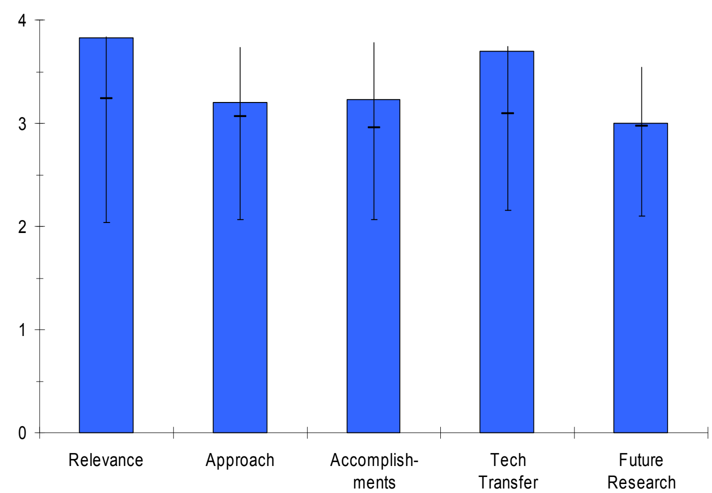
Project # STP-29: Effect of Trace Elements on Long-Term Cycling and Aging Properties of Complex Hydrides for Hydrogen Storage
Dhanesh Chandra; University of Nevada, Reno

[Member of the Metal Hydride Center of Excellence]

Brief Summary of Project

The primary objective of this project is to determine the effects of gaseous impurities (ppm levels of O_2, CO, H_2O etc.) in the H_2 on long-term hydriding/dehydriding of complex hydrides, and a related secondary objective is to determine the mechanisms of degradation. Accelerated laboratory tests designed at UNR can simulate these conditions providing insights into the long term reliability of complex hydrides and their precursors. Research in 2007 focused on effects of using industrial hydrogen for 1100 cycles in a Li_2NH-$LiNH_2$ system. Pressure cycling (~500 cycles) using 100 ppm level O_2 impurity in ultra-high purity (UHP) H_2 as well as thermal aging (CO impurity) of mixed phase Li_3AlH_6-$LiNH_2$ have been completed.

Overall Project Score: 3.4 (4 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.8** for its relevance to DOE objectives.

- This project plays an important supporting role toward the DOE's RD&D plan in evaluating and characterizing promising compositions and their response to impurities and cycling.
- Determination of the effect of impurities on hydrogen storage characteristics and stability is a critical part of the hydrogen and fuel cells for transportation program.
- Fundamental understanding of hydride hydrogen storage capacity and physical stability are crucial to meeting DOE durability targets.
- Addressing an important area – role of impurities.
- Component relevant to fundamental understanding: phase transitioning.
- Studying vaporization thermodynamics, which is often overlooked.

Question 2: Approach to performing the research and development

This project was rated **3.2** on its approach.

- The approach and techniques used are very useful and appropriate toward evaluation of aging and impurities. All of the necessary instrumentation and experimental protocol seems to be well-developed and useful in testing materials. These studies, however, could be a bit more focused and thorough. For example, a variety of different 'exposure' conditions and impurty levels should be tested (including reference data) for each composition.
- This project appears to be covering many areas and should be rethought and refocused on the relevant issues at hand.
- Good analysis tools.
- It is not clear how and if the fundamental mechanistic studies will be generalized from the specific hydride systems being studied to other systems.

- Will general conclusions on effects of impurities be drawn from the impurity empirical work? What are the general mechanisms of the impurity effects?
- Needs more theory.
- Use of an array of techniques: Sieverts, in-situ diffraction, microbalance.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.2** based on accomplishments.

- A variety of hydrogen storage compositions (fed from the MHCoE) have been preliminarily investigated using a variety of measurement and characterization techniques. The most relevant compositions from the metal hydride CoE seem to be rapidly transferred to this partner for evaluation and the testing thoroughly and efficiently performed. While, these studies are vital to the eventual application of a suitable hydrogen storage material, their impact could be maximized with a more detailed experimental focus on each composition rather than a rough suvey of many compositions.
- Most of the technical accomplishment appear not impactful to state of the art. The relevance of the appraoch should be considered.
- The effect of CO on hydride behavior is interesting and encouraging. Is the same behavior expected on other hydrides?
- The mechanistic studies are extensive but the relevance gets lost in the data. How do the results affect the direction of metal hydride research?
- Studied numerous systems: alanate-amide, amide-imide, BH_4-based.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.7** for technology transfer and collaboration.

- Impressive communication between experimental partners and this project. Very effective materials selection and communication lines are in place which drive the current and future success of this project. It would also be nice to see promising materials from other CoEs fed to this project.
- A hydrogen producer would strengthen the team.
- Very good collaborations, which are continuously expanding.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- Strengthen focus on individual compositions under a variety of different impurity and cycling conditions in order to fully characterize the durability and impurity tolerances (and resulting failure modes). Likewise, it is important to include reference/control data for each experiment.
- Needs to be focused.
- Important future work includes more interaction with the theory efforts of the MHCoE.
- Experimental future work follows logically.
- Clear path forward.

Strengths and weaknesses

Strengths
- Experimental capabilities are impressive. Focus on evaluating materials in a potential 'on-board' environment is highly valuable.
- Impurity analysis-critical study. Should be expanded to include other trace gases that metal hydride could be exposed to.
- Integrated use of different techniques.
- Strong collaborations with other partners in the Center.

- Strong international collaborations.
- Addressing rarely thought about issues (vaporization of metals in the alanates and BH_4).

Weaknesses
- Needs boundaries of investigation. For example, material cycling and response to impurity are the assigned studies. However, there seems to be a gray area as to the degree to which this project is being used for fundamental measurements and characterization which should be performed elsewhere.
- Research appears defocused. Impurity effects important enough to be entire study. Linkage to center of excellence not well explained.
- Recommend more feedback from theory.

Specific recommendations and additions or deletions to the work scope

- Make impurity effects focus of study.
- A single page with one-line bullets of high-level accomplishments would help the reviewers understand what has been done and the significance.
- Too much data if that's possible. The conclusions/message get lost in the charts for someone who doesn't “live” with the analysis techniques and their output graphs.
- Recommend more feedback from theory.
- None.

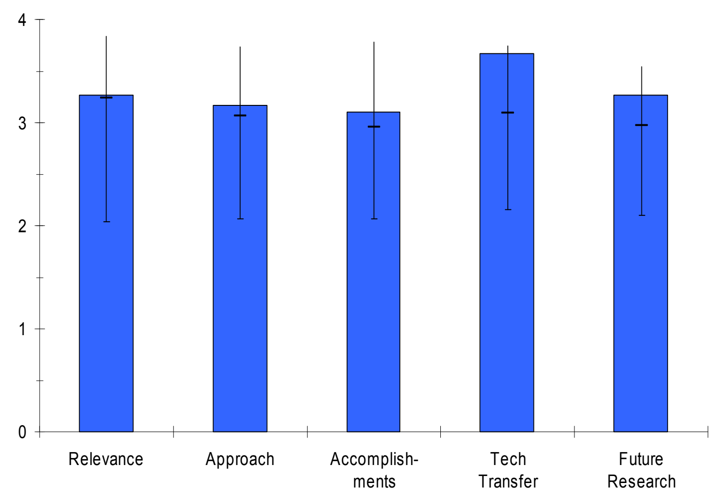
Project # STP-31: Metal Hydride-Based Hydrogen Storage
Ian Robertson (PI), presenting; Duane Johnson (Co-PI); University of Illinois Urbana-Champaign

[Member of the Metal Hydride Center of Excellence]

Brief Summary of Project

The overall objectives of this project are to support and guide development of complex metal hydrides to meet systems requirements by providing center partners with structural and chemical insight of candidate systems and providing experimentally-based and validated theoretical modeling. Specific objectives in FY 2007 are to provide modeling to guide materials development, provide understanding of the role of catalysts, and determine nature, state and effect of surface contaminants on hydrogen uptake and release.

Overall Project Score: 3.2 (3 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

- This MHCoE support project is clearly contributing to the President's Hydrogen Fuel Inititative.
- Project focus is on high-capacity hydrides that need to be optimized to meet DOE targets listed in the Hydrogen Fuel Cell and Infrastructure Technolgies' Multi-Year RD&D plan.
- This project provides direct support of materials development in the metal hydride CoE.
- Project is in a good agreement with DOE objectives.

Question 2: Approach to performing the research and development

This project was rated **3.2** on its approach.

- The effort serves as a miscellaneous support and service vehicle to the MHCoE and thus indirectly helps the "assault" on the many technical barriers to vehicular hydrogen storage.
- PI and his students make important contributions to the MHCoE partners in the form of structural studies, surface chemistry and theoretical modeling.
- It is more a support effort than a lead effort. In that sense, it provides scientific objectivity over competition for a new and revolutionary material.
- This project consists of two relatively independent parts. One is experimental and provides structural and chemical information on metal hydrides. The other part is theoretical, using first principle calculations to determine thermodynamic properties of hydride structures. Both parts interact closely, providing information to each other as well as to the center partners that they are collaborating with.
- This project is not involved in the development of a specific hydride material or system. Both parts provide support to the material development efforts within the CoE.
- Development and maintainance of a structural database is an important contribution to all modeling activities in this center and could be used by other centers.
- University of Illinois's approach is in good agreement with the goals and objectives of the MHCoE and the funding.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.1** based on accomplishments.

- The project is fairly new, but has made several contributions in the first year or so.
- Work has focused on high-capacity materials such as $Ca(BH_4)_2$ and $LiBH_4$.
- Progress has been made in understanding surface contamination; this has led to suggestions for improving kinetics and reversibility.
- Ab initio calculations have confirmed (or not) other calculational approaches within the CoE and other DOE projects.
- A very useful structural database has been created.
- Experimental efforts were focused on borohydrides, including (1) examining rehydriding of Ca borohydride on a microstructural scale; (2) determining non-uniform dispersion of Pt catalysts on Ca borohydride; (3) found uneven distribution of different catalysts on Mg borohydride. These results indicate the complexities involved in determining the optimal fabrication techniques for enhancing hydride kinetics, rehydriding yield, etc.
- Theoretical modeling was mainly directed on Li borohydride: (1) Molecular Dynamics study that determined the high temperature structure and transition enthalpies; (2) DFT calculations that predicted formation enthalpy and P-T curves. Other work examined the reaction of oxygen with LiH as a possibl poisoning reacion preventing re-hydriding of Li alanate.
- The approach used has been tested using relatively simple test system - $LiBH_4$. Whether it would work for more complex ones remains to be seen.
- Chemistry of alanates, borohydrides and metal hydrides is well established. An additional literature search or collaboration with chemists may benefit the project.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.7** for technology transfer and collaboration.

- The project has many useful collaborations within the MHCoE.
- This effort is a very important scientific support contribution to the CoE and could be even more used in DOE projects outside the CoE.
- Excellent collaboration with center partners.
- Collaboration and tech transfer are quite impressive.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.3** for proposed future work.

- The future work is fine. Continue as planned.
- Future work appears to be mainly to continue on the current path by supporting the development of hydride materials by center partners.
- New areas include experimental work examining structure/chemistry of contaminant layers and their role in inhibiting rehydriding, modleing work on kinetics and poisoning issues associated with O+ and OH-.
- Future work looks good.
- A collaboration with chemists may bring additional benefits.

Strengths and weaknesses

Strengths
- The project provides an excellent spectrum of tools to aid the MHCoE partners.
- The modeling activities provide a reality check to other modeling activities within the MHCoE.
- Excellent experimental capabilities in microstructural analysis.
- Excellent theoretical modeling capabilities.

- A good combination of advanced characterization techniques with first-principles electronic and thermodynamic calculations.
- Understanding of advantages and limitations of the approach(es) used.

Weaknesses
- No significant weaknesses.
- A significant part of the future work is "work for others", which may have a negative impact on the final outcome of the project.
- A careful screening of the literature on chemical behavior of light metal hydrides can be advised.

Specific recommendations and additions or deletions to the work scope

- Consider broadening this support activity beyond the MHCoE to other CoEs and non-CoE DOE projects.
- The experimental capabilities of UIUC could be expanded to include more detailed surface science studies of impurity and oxidation effects in complex hydrides and their possible role in inhibiting kinetics and rehydriding. Related work already appears to be in future plans for the modeling effort.
- In-situ studies of microstructural changes during reactions of complex, mixed hydride systems could shed some light on kinetics and intermediate reaction paths.
- A collaboration with chemists may bring additional benefits.
- A careful screening of the literature on chemical behavior of light metal hydrides can be advised.

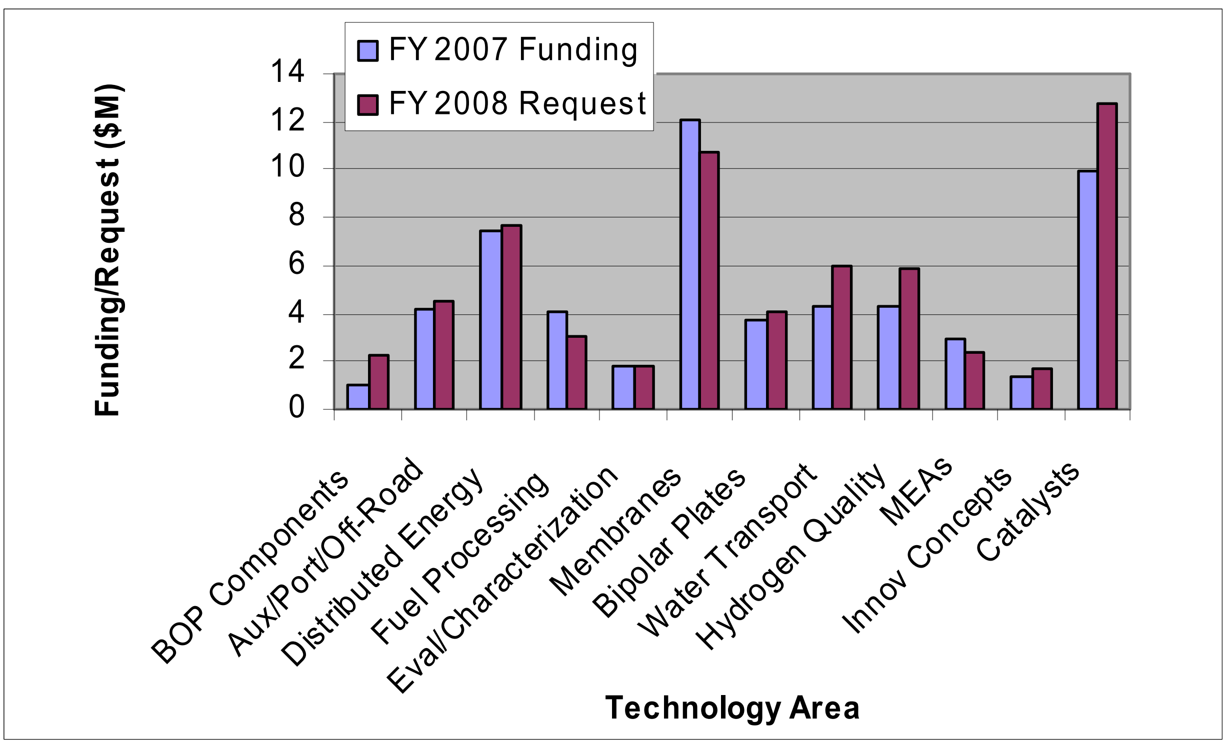
2007
Fuel Cells
Summary of Annual Merit Review Fuel Cells Subprogram

Summary of Reviewer Comments on Fuel Cells Subprogram:

Reviewers consider fuel cell development to be a critical enabling technology for the success of the President's Hydrogen Fuel Initiative. Overall, the R&D portfolio was judged to be well managed, appropriately diverse, and focused on addressing technical barriers and meeting performance targets. Progress was considered good. The current focus on partnering (industry, National Labs, etc.) was applauded and reviewers suggested that some projects might benefit from more interaction with industry, developers, and other program projects to establish a stronger and more technically sound research project with improved outcomes and deliverables. Many R&D projects in the Fuel Cell Subprogram were completed in FY06. New projects from the 2006 solicitation/lab call were kicked off in February 2007 and they were presented in a poster session but not reviewed. As a consequence, fewer fuel cell projects were reviewed this year at the Merit Review and Peer Evaluation. These new projects will be reviewed in FY08.

Fuel Cell Funding by Technology:

The Fuel Cell Technology Subprogram continues to concentrate on the critical path technology of stack components (membranes, catalysts, analysis and characterization, etc.). Cost and durability of stack components continue to be a key focus of the subprogram.



Majority of Reviewer Comments and Recommendations:

In general, the reviewer scores for the fuel cell projects were high to average, with scores ranging from 3.7, 2.8, and 1.8 for the highest, average, and lowest scores, respectively. The majority of the projects were reviewed by six to seven reviewers. The scores reflect the technical progress that have been made over the past year, relevance to the DOE Hydrogen Program, technical approach of the project; extent of technical transfer; and proposed future plans for the project. Key recommendations and weaknesses are summarized below. DOE will respond to reviewer recommendations as appropriate for the scope and coherency of the overall fuel cell research effort.

Catalysts: Scores for catalyst projects received an overall rating of average, but they were rated above average in the categories of relevance to the DOE Hydrogen Program and technical approach. The durability results from the non-precious metal catalyst projects are promising, but performance needs to be an order-of-magnitude better before this durability matters. The reviewers commented these efforts in alternative electrocatalysts represent a potential high pay-off option and should be supported in the future.

Membranes: The membrane projects were ranked average to above average. Virginia Tech and Colorado School of Mines ranked the highest among membrane projects. The use of heteropoly acids for proton conduction in membranes is a novel concept with high potential. A major issue continues to be immobilization of "polyPOM" in polymer materials. The Virginia Tech effort provides a new approach to formulate fuel cell membranes and showed significant progress in conductivity and swelling reduction. A cost of production study of most promising membranes was recommended for many of the projects. One outcome of the 3M stationary membrane activities is the correlation of lifetime with initial fluoride release rate that may enable a lifetime prediction capability.

Recycling: Two recycling projects were evaluated and each received an overall rating of above average. Pt (PGM) recovery is an important aspect of the overall fuel cell life cycle because it addresses both environmental issues and cost issues that impact the cost of fuel cell systems. BASF has made significant progress toward identification of the most efficient processes to recycle both CCMs and MEAs. Significant progress has been made by Ion Power in economic analysis and prototype process demonstration but more cost analysis is needed. BASF should implement a go/no go decision point before proceeding to build a recycling plant prototype.

Stationary: One stationary project (Battelle) was evaluated and its total score is above average. The data collection and analysis methods were considered thorough and systematic. Through the forklift market study, a good tool was developed for future implementation into different market segments. However, all costs to transition and operate new forklifts and other systems need to be included. The data and model from this project will be available to the public to promote technology transfer.

Analysis and Characterization: These projects were ranked average to above average and were noted to strongly support the fuel cell program objectives and goals. The NIST Neutron Imaging Project received the highest score throughout the entire fuel cell program. Correlating microstructure of MEAs with performance data would increase the value of the ORNL TEM characterization effort. Components such as membranes, GDLs, and catalysts from a working stack should be considered for study. The modelers in the fuel cell program were encouraged to validate their models with real world data, as previously suggested. Fuel cell manufacturers need to supply more experimental data to the modelers.

Portable Power, Auxiliary Power, BOP, and Fuel Processing: No projects in these technology categories were included in the Annual Merit Review and Peer Evaluation this year. Projects of this type were on hold and not funded until the middle of FY07.

Bipolar Plates: No bipolar plate projects were reviewed in the Annual Merit Review and Peer Evaluation this year. Two new bipolar projects were included in the poster session but they were not reviewed.

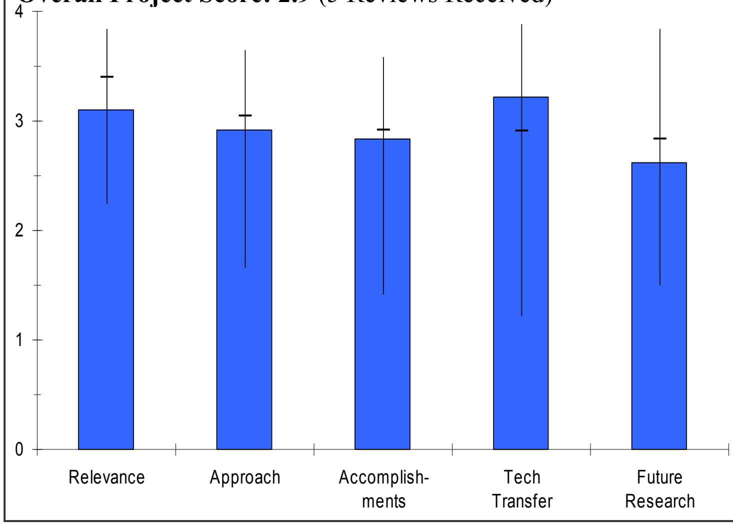
Cross Cutting: One cross-cutting project (National Center for Manufacturing Sciences) was rated with scores ranging from average to below average. The reviewers recognize the importance of manufacturing research and development in attaining cost targets for PEM fuel cell vehicles. Cost data and technical accomplishments must be presented in order to track progress in relation to cost targets and technical goals.

Project # FC-01: Fuel Cell Systems Analysis
Rajesh Ahluwalia; ANL

Brief Summary of Project

The objectives of this project are to 1) develop a validated system model and use it to assess design-point, part-load and dynamic performance of automotive fuel cell systems; 2) support DOE in setting and evaluating research and development goals and research directions; and 3) establish metrics for gauging progress of research and development projects. The objectives for FY 2007 were to develop, document and make available versatile system and analysis tools consisting of GCtool (stand alone code) and GCtool_ENG (coupled to PSAT). The models were then validated against data obtained in laboratories and at Argonne's Fuel Cell Test Facility. These models may then be used by those of current interest, including FreedomCAR Technical Teams and DOE contractors.

Overall Project Score: 2.9 (5 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.1** for its relevance to DOE objectives.

- Project, while not directly vital to the Program's success, provides a useful check on the progress towards the final objectives (such as system efficiency and cost) and warrants continued support.
- Provides operating conditions, strategies, models and insight that can assist and guide other Program projects. For example: models are used for Program's cost studies, water & thermal management project, and air compressor projects.
- Understanding of system-level implications is critical to understanding of DOE high-level targets and to prioritization of specifications/development tasks for R&D.
- A purpose of this project is to create a "paper" fuel cell system in order to provide quantitative insights into fuel cell engineering. ("Paper" in this case means a computer model that simulates an actual fuel cell system in intent if not in practice.)
- This project could be valuable, potentially, as a resource for discovering engineering data that are inconsistent with other data.
- The work is directly relevant to the President's Initiative.
- The work supports the fuel quality work and will help extrapolate the cell data being generated by LANL, HNEI, JARI, etc. to evaluate the effects of changes in cell design and catalyst loadings.

Question 2: Approach to performing the research and development

This project was rated **2.9** on its approach.

- Generally a solid approach, but would benefit from more validation.
- Perhaps too much extrapolation of some models (e.g., membrane water uptake and conductivity at temperatures higher than available data, CO limit outside data range). Again, please validate.
- Modeling work needs to address durability and failure root causes better.
- MatLab compatibility is a good choice for wide usability.
- The absence of uncertainty (sometimes called "error") analysis is a significant weakness. The data used to build the model should have an indication of the uncertainty of the data – perhaps the standard deviation of a

distribution if a result was arrived at statistically. This information should be preserved and propagated through the model in the standard fashion to provide error bounds for predictions of the model.
- The concept of collecting and compiling the open literature test data in one area would be very helpful.
- Using the working model to complement the efforts of NREL and LANL is a plus.
- Is the model to be used to make extrapolations that will later be validated by LANL, HNEI, JARI, etc?

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.8** based on accomplishments.

- The project has delivered on their objectives. Program "barriers" do not apply to this system-based model development.
- Durability prediction is just scratching the surface. Funding level is not consistent with major effort required in this area.
- Decision to use 3M NSTF catalyst and PFSA membrane as reference system may limit applicability of results (for instance water transport, optimum operating temperature) to other MEA/Catalyst systems.
- Not clear that any breakthroughs are being enabled by this activity. Incremental progress towards goals, which are better addressed by developers.
- The purpose of the project is to provide quantitative insight to members of the fuel cell development community. Lacking in the project is feedback from the community as to how this insight affected their decisions and how their ultimate experience compared with the initial predictions.
- The measure of technical accomplishment would be how well the model compares with real-world experience. Some of the slides (e.g., 16-19) make interesting predictions, but without comparison of theory with experimental data, one cannot tell how great the accomplishment might be.
- The model is timely for the hydrogen quality effort, which is a key point in the evolution to a hydrogen infrastructure.
- The evaluation of the 3M membrane and catalyzing technique is helpful.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.2** for technology transfer and collaboration.

- Good interactions with other Program projects (TIAX cost study, Honeywell BOP programs, H_2 quality programs) and FC Tech Team.
- Future work includes durability models. Perhaps this can be tied into LANL's continued durability experimental effort.
- Good interaction with component developers
- Explore use of test data from other test labs (universities).
- Unclear that the developers are using the model, or that DOE is using input from model to revise/prioritize specifications of components or materials.
- The project has many industry partners, which is one of its greatest strengths.
- The project could be strengthened by additional feedback from its partners – how model influenced decisions, how model comported with real-world results, and how model was refined based on such information.
- The interaction between ANL and 3M appears to be very good.
- The use of LANL and U of SC data also appears to be very good.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.6** for proposed future work.

- The future research plan correctly includes developing models and understanding derived from the Program's impurity studies (H_2 quality and air impurities). I strongly recommend focus on impurity effects on reduced catalyst loading electrodes that are required for FC commercialization.

- Systems analysis and hydrogen quality support activities are poorly defined. Need to focus on specific deliverables.
- End-of-Life modeling is potentially a very useful task, but details are missing. Scope of EOL modeling is probably inconsistent with available funding for 2008.
- Future work is primarily support/exercise activity, not directed research towards system simplification or component specification.
- Proposed future research includes new models for end-of-life analysis and fuel impurities. The PI does not explain how building such models would affect the course of the research program to overcome technical barriers.
- The proposed future works makes sense and is relevant. Specific examples would have been helpful.

Strengths and weaknesses

Strengths
- The project has solid modeling expertise.
- Good stack and system mechanical system simulation. Materials behavior and electrochemical behavior prediction needs more work.
- Good collaboration with developers and suppliers.
- Distribution of model should help industry make consistent projections.
- Captures much of the relevant physics for traditional system, steady-state operation.
- The PI cites several collaborators, though it is unclear if they use the model for engineering or rhetorical support (e.g., in PowerPoint presentations).
- The start of using lab and field data from multiple sources.
- The start of using the model to support other efforts like fuel quality.

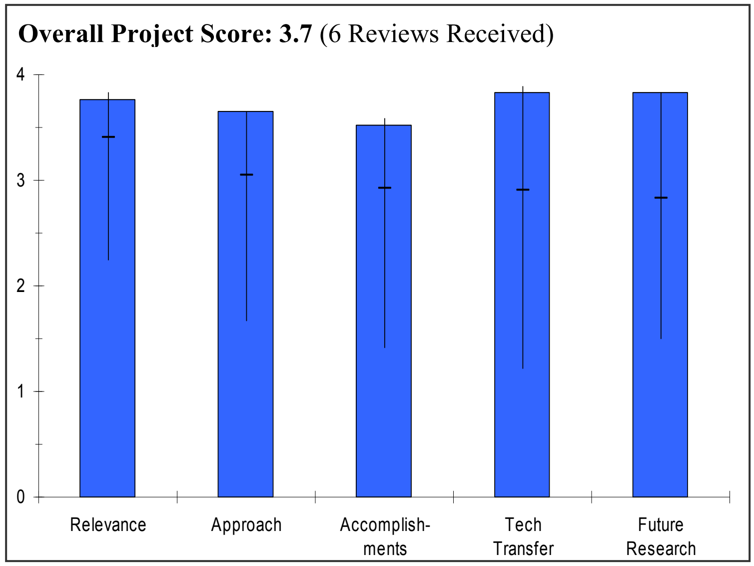
Weaknesses
- The project will still benefit from increased validation of results, especially on potential impact of impurities.
- Many in the audience were confused by the impurity results shown as a function of "recycle ratio". As the PI no doubt is aware, the actual driver was the H_2 purge rate. This would be communicated more clearly if it was referred to as such (perhaps defined as purge H_2 rate/electrochemically-consumed H_2).
- Durability prediction needs to be strengthened.
- This is primarily a paper study.
- Insufficient emphasis on game-changing configurations (elimination of major components or simpler control algorithms).
- Transient phenomena?
- Apparent use of the same sets of data to both create and to validate the model, thus confusing validation with data fitting. This weakness could be corrected by more clearly identifying the sources of data, showing that separate and independent sources were used for model construction and validation.
- Absence of uncertainty analysis. This weakness could be corrected by more clearly showing error bars in the data used to construct the model and confidence bands in the model predictions.
- Lack of demonstrated impact. This weakness could be corrected by showing that the model had value in influencing engineering decisions, correctly predicting real-world experience, or critically evaluating inconsistent data sets.
- Objectives that stress management goals (setting goals, establishing metrics) rather than engineering goals (making accurate predictions, reducing the need for expensive experiments). (One does not need a computer model to "gauge progress of R&D projects" or to "set and evaluate R&D goals and research directions.")
- The apparent lack of validation of extrapolation of the model.
- The leveraging of complementing activities from projects would be an asset.
- As an aside, the presentation has a number of acronyms (e.g., CEM, ORR, EWH, etc). A page defining the acronyms would be helpful.

Specific recommendations and additions or deletions to the work scope

- Prioritize impurity modeling. Hydrogen side followed by air side.
- System model should be used to determine how a change in material or device specification could allow for major changes to system complexity or control.
- Need focus on transient designs/off-design points, which are harder to get data for in power plants.
- Is a comparison of the 3M materials to the DuPont and Gore materials envisioned?
- Does ANL plan on only using the published LANL and U of SC data, or include the data being generated by HNEI, JARI, Clemson, U of CT?
- Has ANL considered requesting these labs to run specific points to validate the model?
- Are alternate cell designs/materials going to be modeled?
- What type of radiator is being modeled? What would be the effect of modifying the radiator design?

Project # FC-02: Neutron Imaging Study of the Water Transport in Operating Fuel Cells
David Jacobson; NIST

Brief Summary of Project



This project aims to develop and employ an effective neutron imaging based, non-destructive diagnostics tool to characterize water transport in proton exchange membrane (PEM) fuel cells. The objectives for FY 2007 are to 1) form collaborations with industry, national laboratories, and academic researchers; 2) provide research and testing infrastructure to enable the fuel cell/hydrogen storage industry to design, test and optimize prototypes to commercial-grade fuel cells and hydrogen storage devices; 3) make research data available for beneficial use by the fuel cell community; 4) provide a secure facility for proprietary research by industry; 5) transfer data interpretation and analysis algorithm techniques to industry to enable them to carry out research more effectively and independently; and 6) continually develop methods and technology to accommodate rapidly changing industry/academia needs.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.8** for its relevance to DOE objectives.

- PI developed tools that are useful for fuel cell developers.
- The benefits of the project are not clearly quantified.
- Very relevant as this technology and future advancements will be critical in solving the water management-stack issues.
- The project is critical to the design of components in which water management is key.
- This tool offers insight into water management within PEM fuel cells.
- Does not offer direct impact, but it can provide insights that may result in important improvements.
- This project is relevant to the DOE program. The development and use of new techniques to characterize fuel cell components and systems that provide complementary data to that available from other techniques is important. The presentation showed nice results from GDLs.
- NIST neutron imaging work is highly relevant to the DOE program objectives.
- Being able to visualize water movement and transport within an operating fuel cell is important in developing a better understanding of the conditions inside a fuel cell.

Question 2: Approach to performing the research and development

This project was rated **3.7** on its approach.

- Neutron scattering has been the most effective approach for *in situ* water transport study.
- The tools are clearly being widely used, but it was not clear how the work impacted the programs of collaborators.
- Most significant advancement in analytical non-destructive testing in many years.
- Facilitating better resolution and cross-sectional analyses to study water is appropriate.
- NIST has a dedicated beam line for neutron imaging of fuel cells and fuel cell components.
- Tomography and radiography are used to image the cell, the latter being emphasized allowing transient data to be collected.

- The use of modeling is enabling more powerful interpretation of their results.
- Have shown excellent results, to date, however further elucidation will require improved resolution, which is planned.
- Project is to make neutron imaging available to the fuel cell community and to facilitate taking and analysis of the resultant data. The new cell designs and data acquisition techniques will enable more efficient use of this facility to generate data. It would help in the future if the presenter indicated the ultimate sensitivity and resolution capabilities of his experimental setup.
- The approach that NIST is taking to grant access to the neutron source is good, namely externally reviewed proposals selected by a Program advisory committee.
- Improving the capabilities of the facility in anticipation of the needs of the user community is very good.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.5** based on accomplishments.

- It was not clear how the data collected agree with expectations based on literature or modeling.
- There was no explanation for the knee in the through-plane water gradient.
- Outstanding – the new detector and the new beam line are evidence of the accomplishments from this group.
- The new detector predicted to be available this fall will enhance this technique even further.
- Would like to see more publications – but this is not a NIST issue, it is a user responsibility.
- They have achieved a 10x improvement in spatial resolution.
- A 40% reduction in time-of-measurement has been achieved.
- Radiography is being used to study stacks with temporal resolution.
- Showed a lot of interesting results in the past year.
- A lot "bang" for DOE's bucks here.
- The use of neutron imaging to characterize water transport will provide much needed information. This effort was relatively new and did not have many results so the presentation came across as a bit naïve. As this program progresses, it should generate a plethora of new results.
- Significant progress appears to have been made since the 2006 AMR.
- Spatial resolution was improved to 25 μ and NIST expects another factor-of-two improvement this fall.
- The addition of a freeze chamber is an important accomplishment for 2007.
- Increasing the intensity of the neutron beam is also an important accomplishment because it reduces the time for imaging to the same resolution.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.8** for technology transfer and collaboration.

- The NIST tools have been widely used and NIST has developed tools to meet collaborator's specific needs.
- Excellent.
- At least 50% of the beam time is being used for non-IP research.
- Allowing excellent collaboration with both universities (via peer reviewed beam time requests) and industry.
- The number of collaborators is very impressive.
- Effort appears to be in its infancy. To ensure the best use of this facility, the PI needs to take additional steps to ensure more researchers know that the facility is available and its capabilities.
- Collaborations are in evidence. About half are for proprietary collaborations and half for open collaborations.
- Open collaborations advance the science of fuel cells to the benefit of the entire community.
- Proprietary collaborations may actually advance the technology even faster than open collaborations but benefit only one company or a small group.
- The balance of proprietary and non-proprietary work appears to be right.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.8** for proposed future work.

- Sound future plans include going to higher resolution, utilizing AC impedance and freeze studies.
- If appropriately equipped, the PI should include some modeling to compare to data.
- New detectors to enhance the resolution are the most important "next step" in which this group could engage.
- New techniques.
- Spatial resolution down to 1 micrometer.
- *In situ* conductivity measurements by EIS.
- Freeze/thaw studies.
- Additional imaging using cold neutrons.
- Very good; proposing useful future steps.
- A reasonable path forward was presented which is dependent upon outside users expressing interest in using the facility. The addition of cold neutrons, with enhanced water sensitivity, will improve the quality of data available using this suite of techniques. The planned freeze/thaw studies provide interesting data.
- Greater resolution down to less than 1 μ will facilitate the study of water formation and transport within the electrode structure.
- Freeze chamber studies are very important to understand the damage mechanisms at work during freezing conditions.

Strengths and weaknesses

Strengths
- The PI has met user demands.
- The PI has shown continual improvement of methods.
- Team is strong.
- Collaborations excellent considering this is outside the DOE.
- Commitment is there at the NCNR.
- State-of-the art world class facility being funded by a Federal/private partnership.
- Excellent.
- Unique tool with interesting capabilities and results.
- Continuous improvements in resolution and capabilities (e.g., freeze).
- Demonstrating the challenges of water management in traditional PEM fuel cells.
- Application of new techniques to fuel cell problems.
- NIST has the capability to assist researchers to achieve the maximum value from the available beam time by training/assisting researchers in operational techniques and by assisting in data analysis and interpretation.
- The use of internal NIST support to increase the resolution down to sub-micron level is admirable.

Weaknesses
- There was no demonstration of a fundamental understanding of the impact of materials on water vapor transport i.e., lots of results but few explanations.
- There was no validation of results with models or literature data.
- None but it would be valuable to have an independent fuel cell expert engaged with the non-proprietary activities in the development of the technique.
- The following are minor.
- Modeling needs to be strengthened it appears to lag behind the experimental work in terms of quality.
- EIS may be too slow to get time-resolved proton conductivity while imaging, it might be better done ex-situ with reference to a few *in situ* well defined points.
- Not a lot of this work has been published in the literature yet.
- Half the requests for beam time are not able to be accommodated.

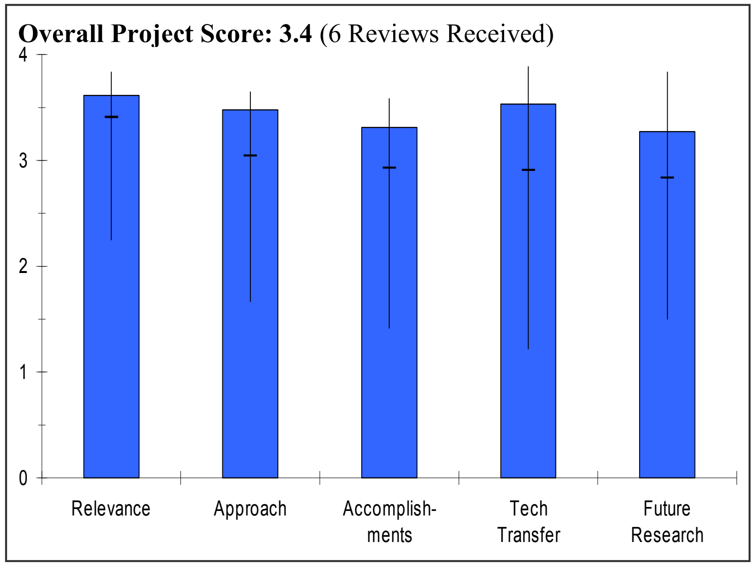
Specific recommendations and additions or deletions to the work scope

- Compare results with models or literature data obtained by other methods.
- Work to differentiate between vapor phase and liquid water.
- Increase the funding.

- Bring in a fuel cell expert.
- Obviously we need more of this, but it sounds like this beam line is maxed out. If possible, provide more beam time.
- Take "snapshots" during freezing process (to capture water movement) and during start-up (if possible) from freeze.
- The project needs to investigate new routes to advertise its existence. The addition of an additional project to investigate transient phenomena during startup, shutdown, and load-following would be beneficial.
- Are there any other strategies to increase productivity of the neutron source so that more requests for beam time can be accommodated?
- Three-dimensional effects are likely to be important in larger fuel cells so the ability to visualize water transport in three dimensions is important. Some effort is justified in trying to develop appropriate imaging technology that can be implemented at the NIST facility.

Project # FC-03: Microstructural Characterization of PEM Fuel Cell MEAs
Karren More; ORNL

Brief Summary of Project



The objectives of this project are to 1) identify high-resolution imaging and compositional/chemical analysis techniques for characterization of the material constituents comprising proton exchange membrane (PEM) fuel cell membrane electrode assemblies (MEAs); 2) apply these analytical and imaging techniques for the evaluation of microstructural and microchemical changes to MEA materials during life-testing; and 3) elucidate microstructure-related degradation mechanisms contributing to PEM fuel cell performance loss. The objectives for fiscal year 2007 were to develop innovative methodologies to prepare samples for microstructural analysis of MEA constituents; apply state-of-the-art electron microscopy techniques for the analysis of MEA materials; and collaborate with industry, academia, and national laboratories to make these techniques available for MEA processing and/or life-testing studies.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.6** for its relevance to DOE objectives.

- PI has demonstrated capability in providing key diagnostic and analytical support necessary for the critical assessment of MEA materials under development by other program participants.
- Very relevant and timely.
- Project is addressing the critical failure modes.
- This project will support the MEA durability and cost effectiveness that are relevant to the Hydrogen Program vision and the DOE objectives.
- Should be very relevant, but the amount of conclusive results produced here appears quite limited.
- The investigator has developed a technique that can be used for quantifying the degree of order in catalyst particles, which can be used for correlations with performance and degradation.
- The project has confirmed known degradation trends (e.g. faster decrease of catalyst surface area at higher RH).
- Identifying characteristics that are stressors for degradation is crucial towards meeting the lifetime targets in the FreedomCAR Fuel Cell Technology Roadmap.
- Using the knowledge obtained from this project can accelerate fuel cell technology developments by eliminating efforts on non-ordered catalyst particles.
- The development of investigative techniques and the determination of lattice structure of alloyed catalyst are relevant.
- The determination of the degree of catalyst agglomeration with time is also relevant.

Question 2: Approach to performing the research and development

This project was rated **3.5** on its approach.

- PI's diagnostic examples were thorough and clearly presented.
- PI's examples demonstrated the relevance of the chosen analytical techniques to the requested tasks.
- Approach is unmatched anywhere and invaluable.

- She is using the most advanced microscopy tools available and leveraging the National Lab resources very well.
- The project integrates with other research areas in the catalyst and electrolyte polymers development fields.
- Further analysis of the technical barriers and system parameters were expected.
- The project's technical feasibility will be greatly enhanced with design modification to include correlations between the catalyst microstructure and its electrochemical performance.
- Need to characterize the changes to the carbon support, as well as the changes in catalyst. For example, the effect of RH on the surface area losses may be (directly or indirectly) due to degradation of the carbon supports.
- If ionomer on the carbon is problematic, then consider some alternative techniques (e.g., is it possible to remove ionomer with alcohol solution?).
- The project is simple and elegant in concept – it focuses on a very important technique for characterizing catalyst particles (z-contrast imaging), and then proceeds to draw correlations using performance and degradation tests when possible.
- The characterization of catalyst particles following degradation has assisted in understanding the mechanisms of catalyst agglomeration (re-precipitation and coalescence instead of ripening).
- Approach needs to begin focusing on sub-surface characteristics if possible. Questions regarding whether particles represent Pt skins over bulk Pt_xM, and whether the sub-surface ordering is important should be addressed. It is unclear from the presentation whether it is possible for ORNL techniques to explore this.
- The evaluation of the structure of the various alloyed catalyst mixtures will help with the development of robust, durable formulations.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.3** based on accomplishments.

- The quantity and "new" technical content of the PI's accomplishments were affected by changes in the projects being supported.
- PI demonstrated capability to adjust to new demands, and development of new techniques required by the changes to project scopes (e.g., "Microstructural Characterization").
- Very appropriate.
- Addressing the most critical components in an analytical approach but also using solid state chemistry fundamentals to guide her.
- Her continued progress on this over the last year was excellent.
- Hope she does not go off on tangents with the "so many" proposed technical solutions. Focus on the existing MEAs and the most relevant possibilities.
- The project certainly shows progress toward the overall project and DOE goals.
- The technical accomplishments will be more significant if more interaction between the collaborating parties was realized.
- Not much in terms of new conclusions here. For example, superior cyclic stability of Pt-Co has been shown and no real conclusions derived (yet) from the difference in alloy order.
- Establishing the link between performance and particle order is the most important achievement for this project this year.
- Establishing that the mechanism of the particle size increase allows for some particle population in the original particle size regime, is another important contribution.
- Project needs to begin identifying a clear link between catalyst particle order and degradation. There is enough data to hint at such a link, but no more.
- The development of the techniques is very important.
- The mapping and evaluation of Pt-Co is useful. The start of work on other alloys is also useful.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.5** for technology transfer and collaboration.

- PI has demonstrated excellent interaction with industry and national labs.
- The collaborations are well established leading organizations.

- Expand the availability of the user center.
- The project encourages the collaboration with industry, academia, and national laboratories to make the advanced characterization facilities and equipments located at ORNL available for interested users free of charge.
- Assistance with relating the physical and chemical behaviors of catalysts, electrodes, etc. to their microstructure may be provided to the invited users.
- Limited, but understandable due to limited budget.
- This project is entirely dependent upon collaboration for the acquisition of materials, so therefore, the degree of collaboration is high.
- Collaboration is on all levels: industry, academia, national laboratories.
- The collaboration with other national labs, academic labs, and industry is to be commended.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.3** for proposed future work.

- PI should maintain an aggressive interaction with the other project PIs and (continue to) identify projects that would benefit from PI's diagnostic expertise.
- Karren is focused and doing what needs to be done. Driving this activity to fundamental solid state science is where she needs to go.
- Would like to see her use catalyst materials which are not just "conventionally accepted" catalysts from suppliers. Would like to see the use of new catalyst materials from various groups around the country.
- The project plans to establish further collaborations with industries, universities, and national laboratories to support microstructural characterizations of catalysts and catalyst supports, etc. The project, however, does not consider possible alternative paths.
- Not clear, is the intent to work on as-received catalyst (and postulate how different materials affect performance) or is the intent to focus on changes in the catalyst after use in fuel cell?
- While the future work section acknowledges the *post-mortem* utility of the microstructural imaging, there should also be a focus on linking durability to the beginning-of-life microstructural characteristics as well.
- Catalyst support characterization should be expanded beyond carbon. Although carbon may satisfy the stationary market, its ability to satisfy automotive needs is doubtful. Projects that incorporate metal carbides and metal oxycarbides (e.g. FCP-29 at PNNL) should be included in catalyst support characterization.
- The investigators should consider whether their techniques can be used for GDL, membrane, or interfacial characterizations as well.
- The continuation of further collaboration should be commended.
- This effort appears to be to establish ORNL as a center of excellence. If so, this would be wise.
- It would have been helpful to indicate what alloy catalysts ORNL plans to review next.

Strengths and weaknesses

Strengths
- PI has consistently demonstrated ability to provide excellent diagnostic and analytical support to Hydrogen Program projects.
- Talented group.
- Outstanding resources.
- Motivated.
- State-of-the-art microstructural characterization equipment and facility.
- Skilled staff capable of the operation of this equipment.
- Excellent analytical tools available.
- A focused and simple strategy to develop an analytical technique that can reveal information about catalyst degradation.
- Intense collaboration with industry, academia and national laboratories.
- Wide customer base for the information generated: automotive, stationary, portable and other markets.
- Wide acceptance of the fundamental data. The data interpretation is sound and logical.

- This activity appears to be positioning ORNL to support industry using tools that are expensive and often unavailable to the small fuel cell companies. This effort is to be applauded.

Weaknesses

- PI needs to publish work (journal articles), using a "reference material" (i.e., not restricted by IP or other confidential constraints) so that techniques and results can be well documented for future reference. Alternatively, co-publish with PIs that were assisted with the diagnostic and analytical services.
- Most presentations were "invited presentations" with limited availability to researchers not present at the meetings.
- Lack of significant parametric analysis to correlate the microstructures and the corresponding performance of the MEA components, namely, catalyst, catalyst supports, polymer electrolyte, etc.
- PI should stick to discussing the characterization of the materials, since degradation mechanisms and/or impact on performance in the cell are not the PI's expertise.
- Other than alternative Pt alloys (e.g. Pt-W and Pt-Co), the project has not yet evaluated more exotic MEA component candidates. The simple strategy should be preserved, but with a wider expanse of materials. It is understood that this weakness is a function of collaborators, not ORNL.
- Techniques are being developed, but no mention was made of standardized methods.

Specific recommendations and additions or deletions to the work scope

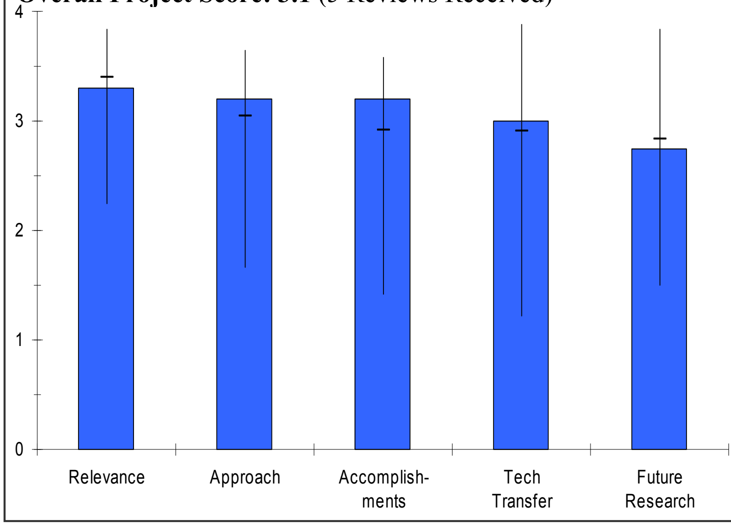
- Suggest that the PI develop a plan to further make the described techniques available to the industry and national labs. Examples might be workshops, journal articles, contributions to "analytical technique" publications.
- Find a way to keep this funded on a permanent basis.
- Add the possible correlations that relate the microstructure of the various MEA components such as catalyst, electrolyte, supports, etc. to their functionality. This will enhance the quality of this project scope.
- Need to characterize changes in carbon (characterize the complete catalyst system). Continuing to ignore this component will lead to the postulation of incorrect degradation mechanisms.
- On used samples, are different cell locations examined? If not, it should be included. For example, one should look for differences between the reactant inlet and outlet locations; recommend comparing the fuel inlet and fuel exit of the 100% RH cycled sample.
- Sub-surface characterization needs to be addressed.
- The full range of the characterization utility has not yet been fully realized. Other MEA component studies (beyond catalysts) should be attempted.
- A more aggressive pursuit of durability vs. component microstructural order is missing and should be added.
- Is ORNL planning to standardize and publish test methods?
- Is ORNL going to evaluate commercial catalysts?
- Is the data to be made public by website?
- Does ORNL also plan to work with industry members on proprietary formulations?

Project # FC-04: Novel Approach to Non-Precious Metal Catalysts
Radoslav Atanasoski; 3M

Brief Summary of Project

The goal of this project is to develop a new, lower-cost, non-precious metal (NPM) cathode catalyst for replacement of platinum (Pt) in a proton exchange membrane (PEM) fuel cell. The objectives of this project are to 1) reduce dependence on precious metals (Pt); 2) have NPM catalysts perform as well as conventional precious metal catalysts currently in use in membrane electrode assemblies (MEAs); 3) have NPM catalysts cost 50% less then compared to a target of 0.2 g Pt/peak kW; and 4) demonstrate durability of >2000 hours with <10% power degradation. The specific objective for FY 2007 is to produce new, better-performing more durable catalysts and identify the catalytic sites.

Overall Project Score: 3.1 (5 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

- Cost is one of the 2 or 3 major hurdles towards fuel cell commercialization, and the stack precious metal loading is the key cost contributor. Thus low cost non-PM catalysts are a key objective, though a high risk, high gain program.
- This is a novel approach to meeting DOE's goals of reducing platinum loading/cost in fuel cells.
- Working well towards DOE's goals for non-precious metal catalyst performance.
- Is cost reduction of 50% valuable – probably not if the fuel cell will have lower power density (requiring more cells, larger air pumps, etc).
- Project addresses DOE goal of development of low cost non-precious metal catalysts; it is relevant to Hydrogen Initiative.
- Project is not critical to Hydrogen Initiative because non-precious metal catalysts have a long way to go before they find commercial application.
- Finding alternatives to platinum for cathode electrocatalysis may prove crucial to the future of polymer electrolyte fuel cells for transportation applications. This project is relevant to overall DOE objectives in spite of unimpressive performance of the catalysts.

Question 2: Approach to performing the research and development

This project was rated **3.2** on its approach.

- In the future, prioritize performance. Durability is important, but at this stage is secondary to performance.
- This is a very systematic and appropriate approach to development of non-noble-metal catalysts.
- Should investigate further support/catalyst interactions.
- Good physiochemical characterization.
- Modeling with something like density functional theory might be useful in the future to help understand/design better catalysts.
- Approach is well designed – scalable synthetic approaches, modeling and physicochemical characterization complement each other.

- Although far from generating performance of any practical value for transportation applications, this study of HNC catalysts offers a path forward for future development of non-precious catalysts for oxygen reduction.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.2** based on accomplishments.

- This is hard to rate. Progress is significant. Performance appears to be the equal of the best non-precious metal catalysts (about the same as for two other Program-funded projects). However, there is still a long, long way to go in catalyst activity before it would be viable for automotive fuel cell stacks.
- Durability results are promising. But performance needs to be an order-of-magnitude better before this durability matters.
- Significant improvement on performance with catalysts/substrates.
- Very good progress towards program goals.
- Work on support is interesting and could be useful for other catalysts.
- Excellent progress toward durability.
- Significant progress in catalytic activity.
- Amount of peroxide for the best catalyst is still high which makes this catalyst an undesirable candidate for potential application.
- Irrespective of the performance level, which remains marginal, the demonstrated durability of the best catalyst is definitely promising.
- Achieving higher surface area with thermally stable substrates is a nice accomplishment.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- The program performance targets are dauntingly high. For the best chance at achieving them, program participants need to leverage as much expertise as possible. I think they'd benefit from more collaboration between the various projects as well as disclosure of the materials.
- If not already done, I'd recommend independent outside testing of the candidate catalysts.
- Good collaborations with Dalhousie and Brookhaven; other interactions were not as clear.
- Lots of work with universities – helps bring them up to 3M's high quality standard for fuel cell research.
- Catalysts cannot be transitioned because catalyst performance is so poor.
- Close collaboration with universities and national labs.
- It is much too early to evaluate this and other alternative-catalyst projects by how successful they have been at the transfer of (yet non-existing) technology.
- Given rather fundamental nature of research, collaboration with several universities is the right approach.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.8** for proposed future work.

- While durability is required, I think it is a little premature to prioritize when performance is still at least an order-of-magnitude away from being relevant to program goals.
- If not yet done, make materials available to DOE labs and OEMs for independent testing.
- Appropriate to explore stability and identification of active sites.
- Program is over, so proposed future research irrelevant.
- Making determination of the active ORR site the focus of research in the remaining months of the project is the right choice.

Strengths and weaknesses

Strengths
- Very good results.
- Interesting approach and smart separation between catalyst/support effects.
- Would like more fundamental understanding.
- Thorough work to develop novel catalysts.
- Innovative work on supports.
- Successful combination of good management and strong research plan allowed to make significant progress toward durability and catalytic activity of NPM catalysts.
- Novelty of approach, out-of-the-box thinking.

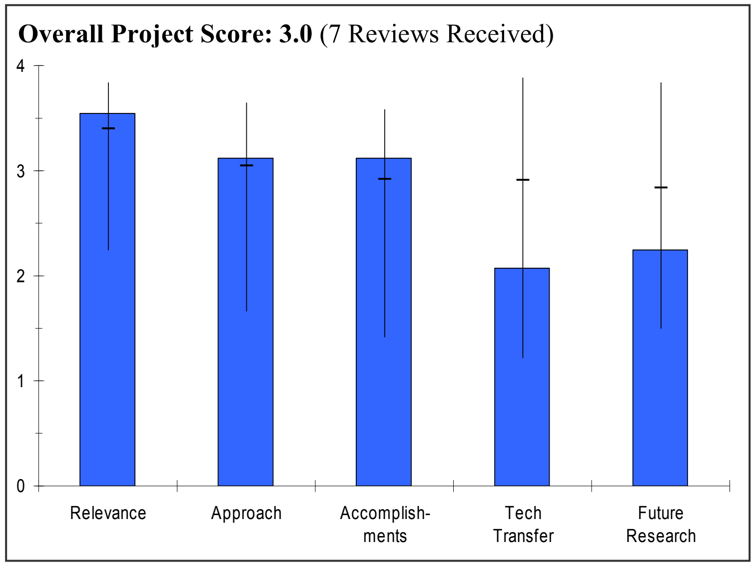
Weaknesses
- Due to poor performance and far separation from targets, would suggest that these non-noble catalysts belong in BES instead of this program in future solicitations.
- Catalysts unlikely to have any practical application.
- The nature of active centers is not determined.
- Unclear how modeling helped in making progress toward discovery of the best catalyst.
- Little insight into the mechanism of oxygen reduction and the nature of active catalytic site.

Specific recommendations and additions or deletions to the work scope

- The stated DOE goals are scientifically challenging but technically irrelevant (e.g. performance @ 0.8 V).
- Performance at high voltages is critical for high fuel efficiency
- Not only relevant to this 3M project, which is scheduled to end in a couple of months: efforts in alternative electrocatalysis, including non-precious compositions such as those demonstrated in this project, represent a potential high pay-off option in oxygen electrocatalysis and should be supported in the future.

Project # FC-05: Novel Non-Precious Metals for PEMFC: Catalyst Selection through Molecular Modeling and Durability Studies

Branko N. Popov; U of South Carolina



Brief Summary of Project

The overall objective of this project is to develop non-precious catalysts for a proton exchange membrane fuel cell (PEMFC) with high catalytic activity, selectivity and durability with a cost at least 50% less than a target of 0.2 g (Pt loading)/peak kW. The specific objectives of this project for FY 2007 are to 1) use metal-free catalysts as a catalyst support; 2) use "metal-catalyzed pyrolysis" to increase the number of active sites; and 3) use chemical post-treatment.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

- Directly addresses low Pt loading targets.
- Cost is one of the 2 or 3 major hurdles towards fuel cell commercialization, and the stack precious metal loading is the key cost contributor. Thus low cost non-PM catalysts are a key objective, though a high risk, high gain program.
- Carbon-based and noble-metal-free catalysts offer potential for substantial cost savings compared to Pt catalysts if activity can be improved. Addresses a major barrier for fuel cells.
- Working well toward DOE's goals for non-precious metal catalyst performance.
- Increasing ORR activity of carbon very interesting and excellent research, but PI should be careful to not imply that this is a useful fuel cell catalyst because activity so low.
- The "holy grail" for reducing catalyst cost.
- A high risk, but potentially high return project.
- Development of a metal-free carbon catalyst provides potential for low cost to meet DOE goals.
- Even if the project is not fully successful, good basic research will provide significant insight for metal catalyst supports and potentially provide cost reduction through more efficient metal catalyst utilization.
- Project supports the DOE goal for development of low cost non-precious metal catalysts for the oxygen reduction reaction.
- Project is not critical to Hydrogen Fuel Initiative due to low activity of NPM catalysts compared to platinum.

Question 2: Approach to performing the research and development

This project was rated **3.1** on its approach.

- Approach is unique and fundamentally sound.
- Stability tests not done at relevant conditions.
- Systematic approach which allowed for the identification of the active site as pyridinic carbon.
- Technical barriers (cost, performance) addressed.
- Approach is largely empirical – impressive that they have made progress this way. Contribution of modeling not clear.
- Something is seriously wrong with the electrochemical evaluation – for instance, on part 6, all catalysts have different limiting currents. Pt/VC catalysts should have a mass activity of 0.16 A/mg Pt at 0.9 V at 25°C at a loading of 14 µg Pt/cm^2 – their performance is negligible at 0.9 V.

- Interesting approach that builds on previous work.
- Work may also result in improved catalyst supports, since it provides insight into the role of carbon.
- Approach modified during course of project based on insight gained from initial approach/research.
- Good fundamental materials research.
- Not clear how well approach addresses cost target.
- Approach is well thought and focused on identification of active sites, improvement of electrocatalytic activity of NPM catalysts and reduction of peroxide formation.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.1** based on accomplishments.

- Continued progress from last year.
- Still very far from meeting DOE activity targets.
- This is hard to rate. Progress is significant. Performance appears to be the equal of the best non-precious metal catalysts (about the same as for two other Program-funded projects). However, there is still a long, long way to go in catalyst activity before it would be viable for automotive fuel cell stacks.
- Most active non-precious metal catalyst developed in DOE programs.
- Decreased peroxide formation to <2% in carbon composites.
- Demonstrated increased durability.
- Identified problems with water management.
- Impressive amount of work on small budget.
- It's hard to evaluate their actual catalyst performance because their RDE measurements are inconsistent.
- PI should list electrochemical conditions (temperature electrolyte rotation rate, reference electrode, current density and disk size).
- USC has done an impressive job improving the ORR of carbon.
- No results presented of molecular modeling at CWRU. Why??
- Good results that also improve understanding of how to achieve good activity without Pt.
- Not clear how much of this was accomplished in the past calendar year.
- Insight into reduction of peroxide formation for carbon catalysts and supports significant contribution.
- Inclusion of baseline (standard) catalyst data on voltage-current plots would be beneficial to ensure consistent measurements done.
- Initial degradation results promising.
- Identification of active sites is a significant accomplishment.
- Tremendous progress toward improvement of catalytic activity and reduction of peroxide formation.
- Modest progress toward durability targets.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.1** for technology transfer and collaboration.

- Little evidence of any collaborative effort.
- The program performance targets are dauntingly high. For the best chance at achieving them, program participants need to leverage as much expertise as possible. I think they'd benefit from more collaboration between the various projects as well as disclosure of the materials.
- Independent outside testing of the candidate catalyst is strongly recommended.
- Collaborations with other universities – could use collaboration with industrial partner or OEM.
- Performance of catalysts is so low that they are unlikely to get picked up by industry.
- Not clear what was done by collaborators.
- Group should be careful to note in publications that these are not practical fuel cell catalysts (yet) and thus not direct more research to low voltage catalysts.
- Appears to be fairly minimal.
- Impact of collaborations not clear without independent knowledge of listed collaborator expertise areas.

- Modeling doesn't appear to play a role in FY05-07 effort – should indicate duration of collaboration if not over full performance period.
- Where does this go from here? No indication of providing materials to cell/stack experts for further validation.
- Close collaboration with universities.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.3** for proposed future work.

- Only recommendation was to find way to add more nitrogen into catalyst.
- Follow through on plan to make materials available to national labs and OEMs for independent testing.
- Project is ending.
- Slightly empirical – not clear why they are focusing on hydrophobicity.
- Issue worth resistance of catalyst layer not explained in talk.
- Only a small amount of funding left – future research somewhat irrelevant.
- Little to no basis provided for how the future efforts in H_2O management, catalyst site optimization, and catalyst layer resistance reduction will be accomplished.
- Based on presented results, appears time to provide materials to group that can address the MEA engineering optimization, since this appears to be beyond the scope of expertise for this performer.

Strengths and weaknesses

Strengths
- Strong structural characterization work.
- In the future, prioritize performance. Durability is important, but at this stage is secondary to performance.
- Have developed an understanding of non-PM catalysts and identified active sites.
- Best activity of non-PM catalysts.
- Innovative basic research – studies of C=N ORR activity might be generally useful.
- Work is structured to attempt to elucidate mechanisms, instead of just trying different materials.
- Work may also result in improved catalyst supports; good opportunity for useful "spin off".
- Concerned about how much peroxide results from alternative ORR catalysts.
- Good understanding of history of this "holy grail" objective.
- Strong fundamental materials research that is providing good insight for future catalyst and support developments.
- Focus on identification of active sites allowed to change directions from transition-metal catalysts to metal-free catalysts.
- Fast progress in implementation of new synthetic routes.

Weaknesses
- Lack of data at relevant conditions.
- No benchmark against Pt catalysts.
- Very thick catalysts layers in MEAs.
- Collaborations with industrial partners who might be able to take advantage of this technology is absent.
- It's nice work/research but unlikely to have any practical value.
- Has not (yet) demonstrated the stability of the catalyst to potential cycling (like in automotive application).
- Explanation for flooding of catalyst layers is speculation with no evidence to support (Pt expels water?).
- Difficult to tell what was accomplished in prior year since FY05-07 lumped together.
- Lack of interaction/collaboration beyond limited materials characterization and theory.
- RDE data on different catalysts are not consistent. For example, it is not clear why limiting current on Pt/C is almost twice lower than limiting current on $RuFeN_x/C$.

Specific recommendations and additions or deletions to the work scope

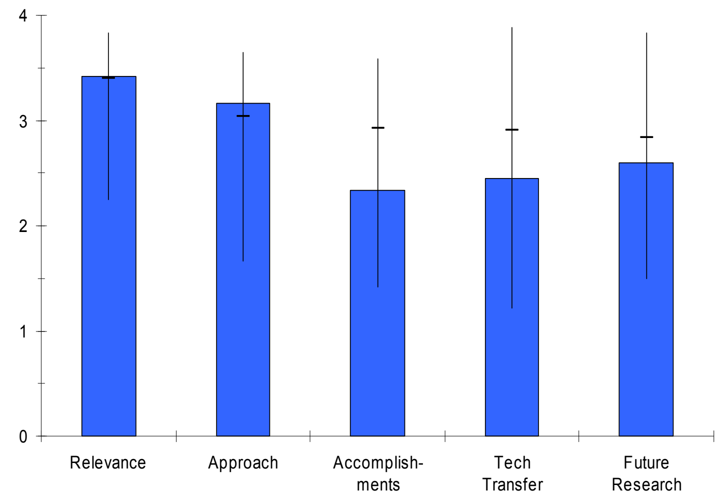
- PI should present progress toward DOE targets.
- Catalyst layers are too thick for reasonable conductivity.
- PI should run DOE-specified durability tests (as opposed to steady state low potential tests).
- Catalysts are not ready for MEA level testing.
- Demonstrate stability to potential cycles (80 hours at steady state is not a durability test).
- Project seems to have reached a natural conclusion barring independent validation of the metal-free carbon and composite carbon material performance and identification of the remaining fundamental issues that need to be addressed.

Project # FC-06: Development of Transition Metal/Chalcogen Based Cathode Catalysts for PEM Fuel Cells
Stephen Campbell; Ballard

Brief Summary of Project

The objective of this project is to develop a non-precious metal cathode catalyst for proton exchange membrane (PEM) fuel cells which is as active and as durable as current platinum group metal (PGM) based catalysts at a significantly reduced cost. The focus of FY 2007 was development of: 1) optimization of the composition and structure; 2) manufacturing process; and 3) evaluation, optimization and demonstration in fuel cell stacks. Materials based on transition metals such as Cr, Fe, Co and two chalcogens (Se and S) were screened for stability and activity for oxygen reduction in dilute acid. Down-selected materials were synthesized as supported catalysts for *ex situ* evaluation as nano-dispersed materials.

Overall Project Score: 2.8 (6 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.4** for its relevance to DOE objectives.

- The development of a low-cost, durable cathode electrocatalyst for PEFCs would be a technology-enabling advance.
- Relevant to DOE goals of platinum loading reduction/cost reduction.
- The purpose of this project was to investigate a class of materials as potential replacement for platinum in the cathode catalyst. This is relevant to DOE objectives by reducing the cost of fuel cell systems.
- Project is relevant to Hydrogen Fuel Initiative; it addresses DOE goal of development of low-cost non-precious metal catalysts.
- Non-precious metal catalysts are very important to the future cost goals in fuel cells.
- Reduction of Pt usage through substitution/replacement is fully aligned with DOE objectives. Non-precious metal catalyst work is very important, even though the probability of success for any one approach is small.

Question 2: Approach to performing the research and development

This project was rated **3.2** on its approach.

- The chalcogen-based catalyst approach is promising and its promise has been demonstrated by several research groups.
- In this project, the promise of a particular chalcogen system was evaluated using sputtered thin film electrodes. A system with promising activity was found, but the PIs were unable to make this particular system in a high surface area fuel cell relevant form. Concurrent development of the sputtered systems and the high surface area catalysts would have allowed the PIs to reach this conclusion earlier in the project.
- Comprehensive approach with thorough characterization of materials.
- The PI adopted the staged approach of evaluating the electrochemical behavior of compounds in a well-controlled geometry before progressing to powder systems with geometries that would be difficult to measure.
- Project approach is well-thought and focused on the achievement of high electrocatalytical activity of the catalysts.
- Unclear why W and Ni were chosen as additives to CoS_2 thin films.

- Went for a challenging approach since they knew going in that the catalyst performance would be difficult to measure but I applaud the willingness to take risks and to take a chance on hitting a dead end (or a new opportunity).
- Ballard has done a thorough job of exploring the potential of transition metal/chalcogen based catalysts.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.3** based on accomplishments.

- Significant progress was made during the past year, unfortunately this progress did not translate into a realistic fuel cell cathode electrocatalyst.
- Good characterization of materials, but very poor performance.
- Although well intentioned and well conducted, this project failed to meet its objectives and was voluntarily terminated by the company at a preplanned go/no-go decision point.
- Significant progress has been made toward physicochemical characterization of synthesized catalysts.
- Moderate progress toward overcoming DOE targets on catalytic activity and durability.
- Some progress in the realization the tungsten was not a viable approach and some decent results using the nickel.
- Not totally clear why these materials were chosen over others and if the risks associated with the research would have been materially different with another approach. In other words, if you had it to do over again, would you take the same approach.
- Project added substantially to our understanding of this class of catalysts.
- Unfortunately, due to intrinsic properties of the materials, targets A (durability), B (cost) and C (performance) have not been achieved.
- Showed a lot of different materials and dopants both for thin films and powders. I was, however, left wondering whether all ideas for using these materials as catalysts have been exhausted. Really need to start thinking in terms of where a particular non-Pt group catalyst needs to get to in terms of performance, then look back and see whether any realistic pathways to get there seem possible. One way is to quantify the theoretical number of active sites.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.5** for technology transfer and collaboration.

- The University of British Columbia and Case Western Reserve University were listed as partners, but it was unclear what their contributions were.
- Good interactions with UBC and Case Western.
- Although these catalysts ultimately proved unsuitable for fuel-cell application, the project generated data on transition metal/chalcogen catalysts that might prove valuable in the future. The PI is encouraged to publish the data generated by this research in the open literature.
- No mention of specific activity from Case Western or UBC but backup slides do indicate that some level of resources were used.
- It is typically a good idea to specifically point out university and national lab collaborations during the presentations since other companies may benefit from being able to build on the research with them.
- Need more, though. I would like to see a Gordon Conference type workshop on non-precious metal catalysts for fuel cell applications, with participants including Prof. Jean-Pol Dodelet (INRS-Canada), Dr. Popov (Univ. South Carolina), Dr. Campbell (Ballard), Dr. Alan Hay (McGill), Zelenay (LANL) and Dr. Atanasoski (3M) at a minimum.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.6** for proposed future work.

- Many people will attempt to keep a project going at all costs even if not in the best interest of the program overall.

Strengths and weaknesses

Strengths

- Excellent capabilities and knowledgeable PI.
- A promising class of catalysts was explored.
- Excellent spectroscopic characterization strategy.
- Systematic approach with good eye on go/no-go decision.
- The project generated interesting material-science data on metal/chalcogen catalysts.
- Strong combination of electrochemical and physicochemical characterization.
- Good detailed investigations of the materials chosen for evaluation with complete testing even in the face of likely negative results.
- Test results were clearly shown with corresponding good data and there were no attempts at enhancing the data to make them appear better than they were.
- Very honest review and willingness to say that the research did not work out.
- Good team, with contributors from both the materials fundamentals aspects (university) and developer/implementer (Ballard). Need both to fully exhaust the possibilities of a given class of potential catalysts.

Weaknesses

- The synthesis of high surface area catalysts should have been performed in parallel with the sputtered electrodes to speed up the development of catalysts.
- Disappointing progress, but researchers acknowledged this and appropriately chose not to continue.
- The project did not meet its objectives and was voluntarily terminated.
- RRDE measurements were not performed which does not allow making any conclusions about peroxide formation during oxygen reduction reaction.
- There is no clear interpretation the difference in electrochemical behavior of sputtered films and powders.
- There is no interpretation of changing OCP after cycling potential to 1.4V.
- Nature of active sites is unclear.
- It seems like some of the issues encountered like the ability to react the metals with H_2S could have been known a little sooner and perhaps there would have been a chance to alter the scope of the project and achieve different results.

Specific recommendations and additions or deletions to the work scope

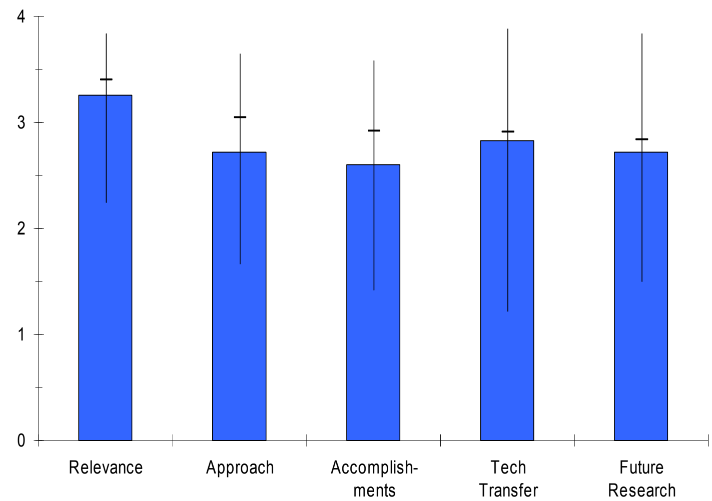
- Not applicable, project is ending.
- None.
- DOE should consider a follow-on solicitation for non-Pt catalysts. Would also need a workshop to define the focus areas.
- I would encourage on all these non-Pt catalyst projects to show results in terms of activity per site and site density (sites/cm^3). Product of these two is A/cm^3 and the target should be 130 A/cm^3. See Gasteiger et al. for details [Appl. Cat. B 2004]. Without a standard basis for comparison across materials families, I cannot tell easily which ones show the greatest promise.

Project # FC-07: Applied Science for Electrode Performance, Cost, and Durability
Bryan Pivovar; LANL

Brief Summary of Project

The objective of this project is to assist the DOE Hydrogen, Fuel Cells & Infrastructure Technologies Program in meeting cost, durability and performance targets by addressing issues directly associated with electrodes. The objectives for FY 2007 for this project are to 1) model oxygen reduction reaction (ORR) using reactive adsorption mechanism; 2) use micro-electrodes and interdigitated microarrays to study ORR and peroxide generation; and 3) to elucidate catalyst utilization and durability of electrodes.

Overall Project Score: 2.8 (7 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

- Maximizing electrode performance, especially the efficiency of the ORR reaction, is crucial for future commercialization of PEMFCs to achieve the necessary power densities.
- Understanding degradation mechanisms and developing countermeasures is also crucial for future commercialization of PEMFCs to achieve the necessary lifetimes.
- This effort is well aligned with the goals and objectives of the overall DOE program.
- The title suggests the work is directed at the top three barriers. The project's focus on understanding better the utilization of dispersed, carbon supported catalysts, however, will only partially support the Hydrogen Vision and DOE R&D objectives, even if successful in finding a way to improve this quantity in a particular way.
- There is much disagreement in the literature as to whether catalyst utilization is as low as suggested by the findings of this work. Major organizations would believe it is at least 80%.
- Carbon-based supports are increasingly being proven not to have adequate corrosion resistance for the durability and tolerance of off-nominal operating events that are characteristic of real life automotive environments.
- The work on understanding ionomer/catalyst interface effects could be of more value.
- Good project that takes a systematic view and is generating some interesting results which may lead to relatively easy improvements (i.e., increasing catalyst utilization is probably easier than developing new ORR catalysts).
- Not clear how this is distinct from other efforts to understand MEA and electrode issues.
- Improvement of Pt catalyst utilization in the electrode is imperative to achieve the fuel cell cost target.
- As for durability, the technical problem is not well defined. Why was hydrogen peroxide formation prioritized?
- Understanding the kinetics of ORR and understanding whether Pt is utilized is crucial to lowering Pt loading and meeting the DOE cost targets.
- Proper measurement techniques for identifying degradation – including measurement techniques – are necessary for meeting component durability targets.
- Peroxide generation is immediately germane to all efforts devoted to extending membrane lifetime.

Question 2: Approach to performing the research and development

This project was rated **2.7** on its approach.

- The PI does not define the specific research topics in a clear and concise manner.

- The PI should clearly state the research topic with target values/results, define the research program to investigate the research topic and provide the current status vs. the target values.
- Lacking direction and focus on key topics – random research attempts on many topics.
- Approach is OK but it would be good to couple this with additional microscopy.
- Such materials changes with time are critical to understand – but, there is more to it than just knowing whether a catalyst particle is in ionic contact. Must also know what the activation energy is for moving a proton from the membrane to the ionomer in the electrode.
- Should focus on ionic transport within the electrode layer to the point where it is understood as a function of water, gas flow rates, current density, etc.
- Optimization of inks and electrode structure is very dependent on the materials and processes used for manufacture, and as such, it is unlikely that this project's use of a 20 wt% ETEK catalyst and their own LANL recipe for making inks will translate to the materials and processes used in MEAs manufactured at volume.
- The use of carbon blacks as catalyst supports should be recognized by this group as fatally flawed and will not be part of the solution in the future and therefore any findings has low probability of translating to help overcome the durability barrier.
- Their very important slide showing how the measured catalyst surface area progressively decreased as the process for forming the electrodes advanced is a clear sign that there are too many variables and process parameters for this project to really discover something fundamentally useful for ink formation.
- Their micro-electrode studies of potential ionomer reorganization at the interface with the Pt catalyst are exciting, (sounds like a potentially fundamentally important phenomenon that has not been appreciated before.)
- The examination of surface area with process treatments is interesting and may lead to novel MEA processes that improve catalyst utilization.
- Lots of little individual but related projects.
- Never connect the dots to address overall electrode issues that are the stated objective.
- More systematic approach is necessary to identify sensitive factors (e.g., operating conditions) with respect to hydrogen peroxide formation.
- Need to identify fuel cell failure mode mechanism led by hydrogen peroxide formation and discuss design and material criticalities to prevent failure modes.
- Need more discussion whether ECSA data can be compared among different measurements. And it is imperative to conclude potential of catalyst utilization (room for improvement).
- The probe into defining the true active surface area of an electrode is the most compelling aspect of this work and it deserves a resolution with some degree of finality and industry-wide acceptance.
- The use of hydrogen sulfide for surface area measurements is creative and enlightening, although a possible nightmare to the more timid safety administrators.
- The use of materials that were more prevalent five years ago (e.g. 20% Pt/C) is a drawback.
- The possibility of hydrogen evolution during hydrogen adsorption measurements should be confirmed to be non-existent.
- Interdigitated arrays helpful for describing the electrochemical peroxide formation.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.6** based on accomplishments.

- Due to the poorly defined research topics, it is hard to gauge the status of the program.
- From what can be understood, the results thus far are good with a potential of high value and content.
- Accomplishments have been moderate in the last year.
- Follows the ORNL concept – need to understand if and how the proton moves within this layer.
- New understandings of the interactions amongst the critical parameters must be focused on and all as a function of the typical environments found within the electrode.
- Differences between the anode and cathode?
- The investigation of ionomer reorganization at the Pt interface is potentially very important, and should be pursued for different catalysts/ionomer structures and conditions.
- Appears to be not particularly impressive for the budget, although this may be more a limitation of the short presentation time at the review.

- All studies cited to indicate Nafion reorganization involve indirect assessment of this phenomenon. Not convincing that this is the mechanism.
- Lots of individual tidbits of knowledge, but not clear how it all comes together to improve electrode performance.
- Well-established measurements.
- At present, the project asks more questions than it answers. Although most researchers have had doubts regarding their electrochemically active surface area measurement techniques, they now have more. If CO stripping or other electrochemical methods are no good, what is? The hydrogen sulfide technique is not meant for *in situ* tests, but yet, surface area measurements are a common metric in accelerated stress tests. If surface area measurements are inaccurate, then why? How might we distinguish area lost by lack of electronic contact from that lost by lack of protonic contact?
- Trends shown with surface area loss throughout the ink and MEA fabrication processes have merit.
- Trends shown with peroxide formation against increasing RH and temperature have merit.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.8** for technology transfer and collaboration.

- High level of collaboration with various universities and national laboratories that are providing very useful insight.
- Lack of a clearly defined program indicates interaction with industry is lacking – while the PI mentions interaction with an OEM, it should be formalized to provide structure to the program.
- Collaborative efforts are good.
- Data is well disseminated to the community as a whole.
- Further interaction with industry would help to select materials better and identify more basic research topics.
- Appears to be minimal (to date), with the exception of the modeling work.
- Any MEA suppliers being consulted?
- Three collaborators listed, but only contribution of ORNL apparent.
- Only seem to be aware of/influenced by what has been previously done at LANL.
- Good interactions for HRTEM and other analysis.
- The ORNL collaboration appeared in the presentation to be more useful for supporting arguments, rather than as part of a proactive development effort.
- The collaboration with Brookhaven to find that PtOH is a dominant surface species is excellent.
- The CWRU collaboration did not have much impact.
- There is still no clear evidence of industry collaboration.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.7** for proposed future work.

- The proposed research to improve the structure of the cathode electrode is poorly defined and difficult to gauge.
- Unclear if the optimization of the electrode structure has already been maximized through empirical research – the PI does not prove it is not.
- Stay the course and continue trying to resolve and answer the questions regarding ionomer-catalyst particles and the impact of electrode architecture.
- I expect greater depth of science from the National Labs.
- Further work on trying to optimize catalyst utilization of the electrode inks should be discontinued because it is not fundamental enough, i.e., it is too process and material dependent and best left to the large scale MEA manufacturers.
- Accelerated studies of the catalyst/ionomer interface should be considered, and include new catalyst structures, not just carbon supported Pt, but alloys and thin film forms of catalysts, to understand how it might influence charge transfer and catalyst surface structure.
- Good plan.
- Proposed kinetic studies are nothing new – what's unique here?

- Lacks scientific/technical basis for how they will correlate performance and structure.
- Lacks systematic approach to identifying characterization methods to develop for future insight – just keep trying things and see what works.
- Not so clear for approach of kinetics study, recommend incorporate modeling approach (e.g., molecular dynamics) to empirical approach.
- Focus on interface of coupling performance is good and useful outcomes are expected.
- The future work indicated is going exactly the direction it should. Catalyst accessibility must be increased.
- Decoupling of electronic and protonic conductivity losses must be approached in the future.

Strengths and weaknesses

Strengths
- Scientific ability of the PI and various collaborators is quite high.
- Understanding and maximizing the electrode structure could provide great improvements in power density values.
- Talented team.
- Resources are well utilized and are excellent.
- Taking a systematic approach to understanding what limits performance (and durability, presumably eventually).
- Empirical approach and measurement tool availability.
- Database development.
- Understanding of technical problems.
- The project demonstrates understanding of crucial electrode issues.
- Creative techniques are used to probe electrode issues (iterative deepening depth-first search algorithm, hydrogen sulfide surface area measurements).
- Reporting of trends involving hydrogen peroxide formation and surface area loss with processing.
- Mathematical modeling with Brookhaven NL.

Weaknesses
- Significant lack of high level project management – research is random and unorganized.
- PI did not sufficiently demonstrate that the work has not already been completed.
- Team seems to be limited in thinking to conventional electrode dynamics.
- Need to concentrate on the evaluation and the science of the interface and electrode layer as to how it impacts the electrocatalytic activity and proton conductivity within this later.
- Appear not to be working with state-of-the-art catalysts (20% Pt on C)?
- Random collection of experiments with no rationale for why they are the critical experiments or best technique.
- Survey of surface area measurements, but appears that they did "what worked for them." No justification for why their surface area number is good – where's the corroborating evidence?
- Systematic approach to identify factors to affect on technical problems.
- Unanswered questions still remaining regarding electrode surface area measurements.
- The project is now in a position where some *in situ* experimental technique must be endorsed for electrode surface area measurements (even if its weaknesses must be acknowledged).
- Lack of industry collaboration.

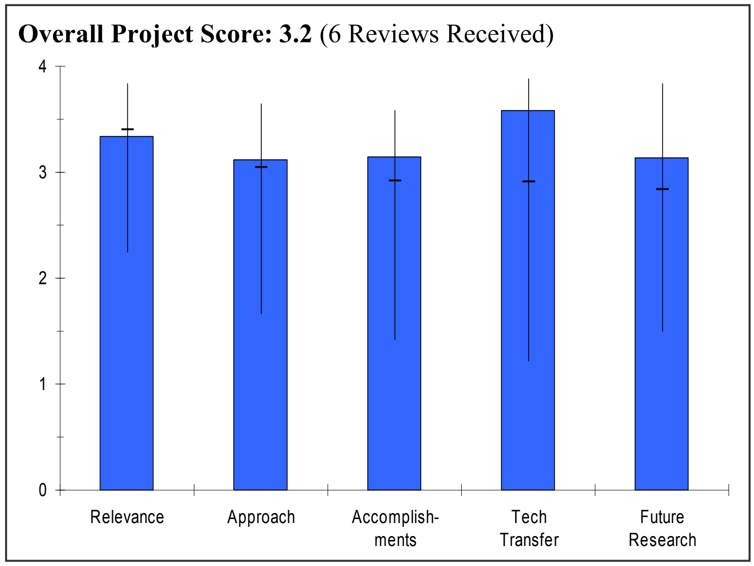
Specific recommendations and additions or deletions to the work scope

- Focus on key topics with a clear definition of targets and research pathway.
- None specifically except for the comments above about the evaluation of the electrode proton transport dynamics in greater detail.
- May want to consider consulting with MEA suppliers to ensure that their assumptions about state-of-the-art MEA processing are correct.
- Use higher wt % of Pt (or Pt alloy) on C.
- After gaining insight into the catalyst utilization and developing some improvements, look at effect on durability, including degradation of the carbon (as well as the catalyst surface area).

- Need to apply and correlate additional characterization techniques to determine whether Nafion reorganization is the appropriate mechanism and to determine how to influence the interactions at a molecular level to improve performance.
- For durability study, pursue the sensitivity measurement to identify factors that affect fuel cell failure before focusing on specific factors.
- Theoretical consideration is necessary to identify improvement room for catalyst utilization.
- The bonding of electrodes to the membrane should be considered for the project scope.
- General Motors has shown work indicating that the structural integrity of the catalyst layer has effects on membrane degradation. Los Alamos could pick up this effort and create a publicly accessible knowledge base on the issue.

Project # FC-08: Development of Polybenzimidazole-based High Temperature Membrane and Electrode Assemblies for Stationary Applications
John Vogel; Plug Power

Brief Summary of Project



The objective of this project is to identify and demonstrate a membrane electrode assembly (MEA) based on a high-temperature polybenzimidazole membrane that can achieve the performance, durability and cost targets required for stationary fuel cell applications. The membrane objectives for FY 2007 for this project are to 1) formulate and characterize polymers; 2) improve membrane mechanical stability; and 3) scale up process and fabricate full size MEAs. The MEA objectives for FY 2007 for this project are to 1) conduct 50 cm^2 screening tests at RPI; 2) conduct parametric tests to characterize fully MEA performance; and 3) assemble and test a full size short stack. The stack objectives for FY 2007 for this project are to 1) characterize acid-absorbing materials; 2) optimize flow fields and sealing; 3) develop novel electrodes using nanotechnology; and 4) perform cost assessment.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

- High temperature stationary stack operation is of high value for the consumer and the nation's energy security.
- The pursuit of stationary applications is in line with the Hydrogen Fuel Initiative, although not as critical for U.S. energy security as transportation.
- Development of a stack for high temperature and dry operation for stationary applications.
- This project is relevant because it is exploring the pitfalls and problems involved in taking the final and usually the most frustrating last steps to a commercial product. Such work, although often seen as work that industry should perform, is necessary to be done in the DOE program, as it provides useful lessons as to how single cell experiments translate into full stack deployment. A weakness of the presentation is that not much detail is provided on what these issues are. More detail on modeling of the stack would have been helpful to aid the DOE's goals.
- The project is clearly focused on a specific approach to meet the DOE stationary fuel cell durability goals.
- Project aligns well to goals of reducing manufacturing costs and improving durability.

Question 2: Approach to performing the research and development

This project was rated **3.1** on its approach.

- Not giving the initial specifications to BASF slowed down the program.
- Overall approach is high with well-defined and clear goals and targets.
- This is a development effort with little research. Tolerances, specifications and lifetime studies are necessary for commercial implementation.
- Graphitic carbon plates. Pt alloy catalyst. Eliminate low MW PBI. Oversized acid trap.
- Burner to eliminate condensation during start up/shut down.
- Approach to this project is good. The program description appears to cover all the necessary factors for successful completion of the program.

- This approach with high temperature PBI/PA is currently the only alternative to low temperature PEM systems and, as such, is good to explore for its effectiveness in this application.
- The approach to develop this technology in a manufacturing facility is good because it clearly shows the issues with integration of MEA and stacks.
- Technical approach is focused on overcoming barriers.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.1** based on accomplishments.

- Durability targets are increasing through membrane, GDL and system design.
- Current densities are still low – unclear how high they will eventually be and whether or not they will achieve a level for commercial success.
- Most of the effort has been focused on tolerance issues with GDLs and getting results to agree with BASF and RPI. Acid migration and trap work is also necessary as well as tradeoffs of temperature studies, but less was accomplished than I would have expected with too much effort just coordinating results.
- 2 MEA failure modes identified – BASF cannot meet specifications on MEA tolerance.
- 10,000 hrs before acid breakthrough.
- Projected 14,000 hrs stack life.
- Generally good progress in most areas. However, there is some concern about the durability and failure. The stacks are failing at fairly short lifetimes relative to the target 40,000 hours and no real cause or plan to discover the cause is outlined. This reviewer does not see how the durability goal will be achieved from this effort.
- Good rate of progress over past year, however, one wonders why the Nafion/PBI mind-set change took so long to be realized, since many of the same issues of compression control, catalyst degradation, etc. are practiced in their low temperature PEM systems.
- Project is nearing completion on accomplishing planned activities and through funding.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.6** for technology transfer and collaboration.

- Technical transfer is high – unclear what the relationship is between RPI and BASF.
- Higher interaction with BASF and Plug will be needed to prevent further slow downs of the program
- Strong collaboration involving people who will likely be responsible for commercialization of this technology, including BASF Fuel Cell, RPI, Albany Nano Tech, Entegris, and University of South Carolina.
- Good to excellent. The RPI work is excellent and the tech transfer issues have been instructive.
- It would seem the past year has been successful in resolving a number of unexpected issues.
- Appears to be good collaboration with BASF and RPI.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.1** for proposed future work.

- Program is almost complete with good success.
- Further membrane/MEA/system optimization will be needed to achieve durability and performance targets – seems to approach with good concepts.
- Project is finishing. No plans for future are given, particularly how to meet the 40,000 hour goal.
- The plans are logical and necessary to fulfill the contract.
- Multiple tasks for 2007 will complete project.
- Need to get MEA cost estimates.

Strengths and weaknesses

Strengths

- Unique technology to Plug, BASF and RPI with the technical leaders in this field.
- General program management appears to be strong.
- Real data and functioning systems.
- Very impressive reduction to practice of a new material.
- Funding should lead to commercialization of technology.
- Excellent demonstration of development problems and how the last few issues could cause a project to fail. The project shows good progress to deal with this.
- It would seem to be the only feasible approach currently known to make a high temperature PEM fuel cell (> 130°C).
- Good record of accomplishment of tasks as project nears completion.

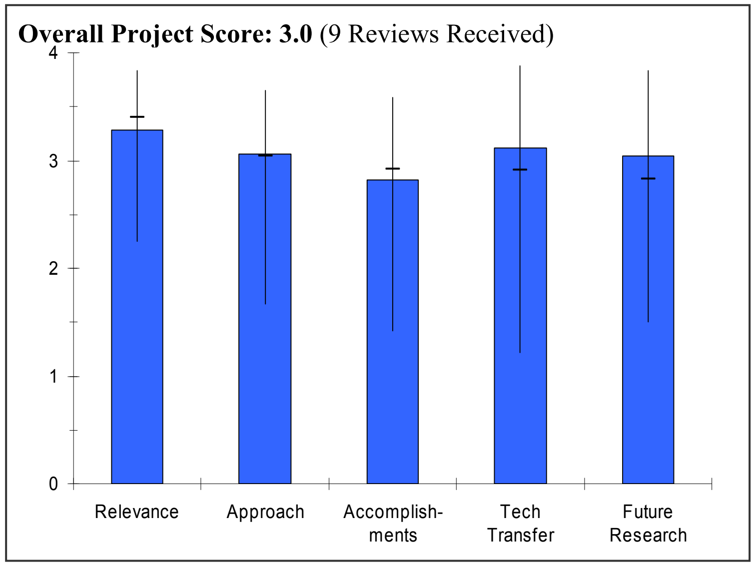
Weaknesses

- Increase communications between Plug Power and BASF to prevent future slow downs of the program.
- Unclear if this technology can achieve the power densities needed for commercialization.
- Unclear is this technology can achieve the cost targets needed for commercialization (low power density will increase the stack cost due to a higher number of repeating units).
- Too much wheel spinning to baseline results between different organizations.
- BASF MEA needs improved manufacturing.
- Project is finishing and future planning not spelled out. Also some of the durability issues do not appear to be understood.
- The market requirements for cost, system volume and complexity may be difficult to meet.
- Still no MEA cost information.

Specific recommendations and additions or deletions to the work scope

- Cost predictions for MEA and system are vital – if predications cannot achieve target values, the need of this program decreases significantly.
- Project concluding.
- Excellent work.

Project # FC-09: Development of a Low-Cost, Durable Membrane and MEA for Stationary and Mobile Fuel Cell Applications
Jung Yi; Arkema Chemicals



Brief Summary of Project

The objective of this project is to develop low-cost and durable membrane and a membrane electrode assembly (MEA) that can meet DOE targets and help drive the commercial reality of fuel cells. The objectives for FY 2007 for this project are 1) the development and characterization of new-generation membranes; 2) MEA optimization; and 3) durability testing of the membrane in fuel cells.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

- The need for increased durability in membranes exists. Membrane cost is not a critical issue for fuel cell commercialization.
- Low cost, high performance membrane electrolytes are an enabling technology.
- This project is aligned with DOE objectives.
- Membranes for multiple applications within program.
- Contributes clearly and strongly to DOE energy independence goals.
- Very limited relevance to DOE Hydrogen goals since the demonstrated technology is coal-to-power.
- Unique approach to lower membrane cost in theory. Need to understand relative costs of full fluorination vs. modifications to make PVDF more chemically stable.
- This project addresses a critical need for fuel cell components.
- Important to go down in cost, but no data shown how to achieve the goal.
- Barriers are consistent with DOE goals.
- Relevant.

Question 2: Approach to performing the research and development

This project was rated **3.1** on its approach.

- Blended membranes have not been as widely pursued as other techniques. PVDF is a known stable, relatively low cost polymer.
- Blended membranes have notoriously poor durability because the driving force for phase separation is large. The lack of any long term morphology characterization or long term performance data is a serious shortcoming.
- More fuel cell data (not just initial performance and OCV tests) need to be presented.
- Decoupling the mechanical and conductivity properties of the membrane through blending of the structural polymer and the polyelectrolyte is an excellent approach which can potentially eliminate the inevitable trade-off between these properties in homogeneous materials.
- Hydrocarbon-based polyelectrolyte may be susceptible to degradation in the extremely oxidizing and acidic environment of the fuel cell.
- The proposed methodology to performing the research work is satisfactory.
- Good mix of materials selection testing and cell-level testing
- Data indicates good performance.
- High-temperature excursions should be at low-RH, not high-RH to mimic real fuel cell operating conditions.

- The approach of an ionomer/Kynar blend may be considered as a way to develop a "reinforced membrane", so the improvement in mechanical properties should probably be compared to a Gore membrane rather than Nafion.
- How much effort or opportunity is there to improve the properties of the polyelectrolyte? What are its fundamental advantages or disadvantages over a PFSA?
- The new generation M41 shows less sulfur loss (but no information how it was achieved).
- Good approach to use composite materials.
- Clear approach to get cost down by using hydrocarbon electrolyte and cheap reinforcement material.
- The PI should comment on compatibility between polyelectrolyte in membrane and electrode.
- H_2/air performance should be tested.
- The ex-situ and *in situ* resistances should be measured at the same conditions!
- The high-temperature excursion test has saturator dew point larger than cell temperature – condensation can occur.
- No low RH measurements → should be remedied → cycling needed.
- Swelling not reported → why? → dimensional stability is key.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.8** based on accomplishments.

- While there is some interesting data, the focus on only OCV and beginning of life tests is a significant weakness for a project focusing on cost and durability. OCV is only a measure of oxygen crossover and peroxide degradation and means nothing for other degradation mechanisms. The lack of lifetime fuel cell data is disappointing.
- High water uptake of these materials also leads to concerns with mechanical robustness.
- Excellent progress in improving the sulfur loss rate and the fuel cell performance from M31 to M41.
- Despite progress, sulfur loss is still high compared to Nafion.
- Substantial improvements since last year.
- Improvement on durability.
- New membranes have been developed/characterized and scaled up.
- MEAs have been optimized and fuel cell testing performed.
- Better mechanical properties and gas permeation than Nafion but lower conductivity.
- Nice adaptation to challenges around interconnect technology.
- Selection of anode catalyst seems to be successful.
- Need to provide information about cost projections (B. Cost Target is critical to program).
- Would like more information about implications of greater swelling in XY direction relative to MEA and seal design.
- Gas barrier properties are very interesting. Would like to compare H_2 to O_2 crossover for understanding of peroxide.
- Chemical stability data is compelling. Why are C-H bonds less susceptible than C-F bonds in Nafion?
- One might have expected the mechanical property improvements over Nafion 111 to have been greater.
- The durability test results look very promising.
- The electrode shorting issues alluded to in the slide on OCV durability testing is a concern since it could compromise the durability tests for both the Nafion controls as well as the project's membrane.
- The source of the electrode roughness should have been addressed in the MEA integration stage.
- What is known about their polyelectrolyte? How different is this from Nafion or standard PFSA?
- Good progress in decreased sulfur loss and achieving therefore a good longevity (even though it was not told how they achieved it).
- The PI should provide polarization data based on H_2/air and not H_2/O_2.
- The drop in performance over 8 hrs at high temperature (high RH) is a matter of concern.
- The PI should provide low RH data → cycling.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.1** for technology transfer and collaboration.

- The team has too little fuel cell experience, and perhaps this is why there have been so few meaningful fuel cell studies reported. No RH cycling, no lifetime performance.
- UTC inclusion on team is beneficial, however it appears that UTC has not been involved in the project up to this point and the project is ending in one month.
- The roles and contributions of the other team members were not clearly stated in the presentation.
- Good collaboration with other entities.
- Universities – Georgia Tech, University of Hawaii.
- Johnson Matthey Fuel Cells.
- No outside collaboration is apparent. Not clear that this impacts achievement of goals.
- Work with material suppliers could speed results.
- Good collaboration with developers at various stages of process (membrane, MEA, stack).
- Would like more information about MEA optimization for different membrane properties.
- Very good selection on industrial participants: Membrane and catalyst manufacturer as well as system integrator.
- Good collaboration.
- Role of Georgia Tech unclear.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- Project concluding.
- The project in its current form is ending and there are many tasks to complete in the very short length of time remaining in the project.
- The proposed plans are consistent.
- Complete durability testing.
- Larger scale fuel cell testing.
- New polyelectrolytes.
- Good cell testing will be critical information.
- Investigation to understand how PVDF can manage similar/better chemical stability in polymer backbone would be critical to understanding not only of this polymer but also other alternative membranes.
- Completing the stack testing at UTC, if it uses their water transport plate system, will prove performance and durability under fully humidified conditions, but not hotter, drier conditions.
- Wants to show lower RH measurements and different load cycling: important.
- RH cycling → step in right direction.
- No comments on dimensional stability → why?
- Lowering of OCV during accelerated testing not addressed → should be.

Strengths and weaknesses

Strengths

- Cheap materials that if stable could find a use in fuel cells.
- Decoupling of the roles of various components of the membrane to optimize mechanical and conductivity properties independent of each other.
- Innovative approach to material development by decoupling mechanical and ionic conductivity properties.
- M31 and M41 have lower cost approach compared to Nafion.
- Kynar technology.
- Good collaborators.
- Good selection of material for anode and interconnect to address challenging operating conditions (carbon, sulfur).

- Nice use of testing to validate material selection.
- Good results (performance, durability).
- Thorough measurements of physical properties.
- Strong technology company with good conceptual approach.
- Variety of polyelectrolytes.
- Chemical stability of membrane seems to be good.
- This membrane leads to better water management.

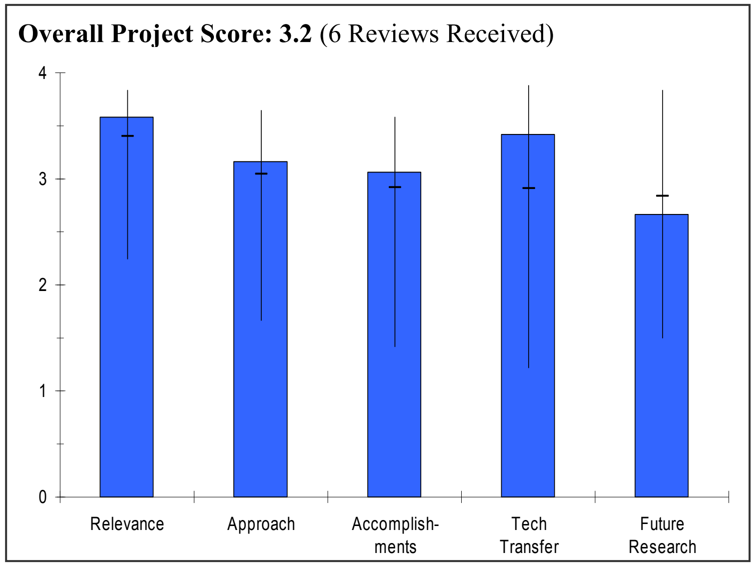
Weaknesses
- No useful data for true evaluation of these materials given. I feel certain that lifetime data must have been taken with these materials and is not reported perhaps due to performance. I'd feel much more comfortable seeing this poor performance and having it correlated with morphology problems than having it completely deleted. Some concerns with temperature stability of these blends might be expected and nothing on this topic has been presented either.
- Degradation of electrode was observed with high temperature cycling. If this effect is due to degradation of the ionomer in the electrocatalyst layer, then developmental effort should focus on improving the stability of this ionomer.
- Swelling is slightly worse than Nafion, and since swelling is linked to degradation, it might have a negative effect on membrane durability.
- Really does not push the envelope in terms of proton conductivity for hotter/drier operation.
- At this point, little advantage over other reinforced membrane technology.
- Collaboration with suppliers and stack integrators could be useful for dissemination of results.
- High-temperature excursions are not realistic at high RH.
- Need to understand fundamentals better, e.g., why the PVDF backbone is stable.
- MEA integration appears to not be emphasized sufficiently.
- Project does not appear to have had a facet dealing with the optimization of the polyelectrolyte.
- No data with air.
- Accelerated tests not comparable to tests done in other projects.
- Unclear how using PVDF as a base will reduce costs considerably.
- Despite chemical stability, durability appears to be suspect as seen from OCV drop.

Specific recommendations and additions or deletions to the work scope

- Project is concluding, but follow-on projects should report more structural characterization, particularly as a function of time in these systems. Lifetime data needs to be presented from fuel cell tests.
- This project is ending in June 2007. Suggestions for the new project are to improve the high temperature stability of the electrode layers and to test the conductivity/performance under low relative humidity, low temperature, conditions and after low temperature cycling.
- Long-term testing higher than 400 hours should be performed.
- Hydrogen-air testing should also be performed.
- Performance tests at low temperatures should be carried out.
- Cost targets should be addressed.
- Arkema should be much more adventurous in their ionomer discovery program.
- The PVDF blend approach is demonstrated but is not useful unless they can improve the conductivity of their materials under hot and dry conditions.
- Need to keep ultimate goal of stack development in focus.
- More fundamental investigations/collaborations with academia to characterize.
- Testing under low-temperature/subfreezing conditions.
- Clarify the uniqueness or advantages of their Arkema polyelectrolyte over more standard ionomers, that is, are there properties that can be improved with this component?
- Include swelling measurements.
- Include H_2/air data reporting (this is a must).

Project # FC-10: MEA and Stack Durability for PEM Fuel Cells
Mike Yandrasits; 3M

Brief Summary of Project



The objective of this project is to develop a pathway/technology for stationary proton exchange membrane (PEM) fuel cell systems to meet the DOE's 2011 objective of 40,000 hour system lifetime. The project goals consist of developing a membrane electrode assembly (MEA) and system with enhanced durability that is 1) manufacturable in a high volume process; 2) capable of meeting market required targets for lifetime and cost; 3) optimized for field ready systems; and 4) capable of a 2,000 hour system demonstration. The focus for fiscal year 2007 for this project are 1) MEA characterization and diagnostics; 2) MEA component development; 3) MEA degradation mechanisms; 4) MEA nonuniformity studies; 5) hydrogen peroxide model; 6) defining system operating window; 7) MEA and component accelerated tests; 8) MEA lifetime analysis; 9) stack testing with intermediate developments; and 10) final stack demonstration.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.6** for its relevance to DOE objectives.

- The program concept is quite relevant and will add to the overall understanding of the critical issues faced by stack developers and systems integrators today.
- The project focuses on durability (40,000 hours) and is in line with the DOE program objectives.
- Durability of fuel cells is a critical barrier, and thus this project is highly relevant.
- Important contribution to durability goals.
- Still no progress on evaluating cost impact, despite reviewer's comments from last year. No data presented to evaluate if this contributes or detracts from cost reduction goals.
- Project focuses on important durability issues. It demonstrates an excellent mix of fundamental science and empirical data collecting and handling in order to predict lifetime. This is critical for DOE to achieve its goals.
- Durability has evolved to be major deterrent to both successful vehicle and stationary fuel cell systems.
- It is very important to the program to have competent and well-equipped researchers like 3M and their partners putting serious efforts into improving durability.

Question 2: Approach to performing the research and development

This project was rated **3.2** on its approach.

- Approach is good yet it seems that too many tasks were signed up for and as the program ends this year, it would have been good to have seen selected tasks developed and the results "used" within this program.
- It is not clear what is driving the effort; is it the stack requirements, the system requirements from the end user, or is it the materials properties?
- Not clear what the stack design and capabilities are and which will impact the MEA – and as well, how the MEA dictates stack designs etc. and how all these are related in this program.
- The project has a good, balanced approach.
- The presented methodology addresses durability very thoroughly.

- Good use of the segmented cell as a diagnostic tool.
- Good use of fluoride ion mapping and membrane modeling to understand degradation modes and identify methods to improve lifetime.
- Good techniques for evaluating mechanism for peroxide degradation.
- Use of model compounds allows team to get a handle on degradation mechanisms and reactions.
- No evidence that capillarity modeling at Case was used in MEA design.
- Not clear from presentation how this work will impact pure H_2 vs. reformer systems.
- Approach is outstanding – chemical understanding, engineering and empirical lifetime predictions that take into account statistical variability. Would like more DOE projects to provide similar comprehensive coverage.
- The approaches for modeling membrane degradation, GDL characterization, and MEA non-uniformity studies appear well-thought out and effective.
- The approach for MEA lifetime modeling is very weak for many reasons, especially a) the combination of log-log plots is not likely to have any value outside the data range and b) with no transients included in the "lifetime" base data, the data (and resulting projections) would not be very robust..
- The testing approach of using only a series of steady-state load conditions is certainly questionable, at least for automotive applications. It is well known that start-ups, shutdowns, and transients dramatically affect durability.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.1** based on accomplishments.

- The accomplishments appear good but it was not easily discernable who was doing what or the significance of the findings. Also, did not see specific accomplishments from the various team members.
- Would like to have seen more data regarding the cell interactions from the segmented cell.
- Would like to have seen start-stops in the testing.
- Substantial progress on development of procedures to identifying membrane degradation mechanisms and operating strategies to minimize performance decay has been achieved.
- Progress on durability is good.
- The project has produced useful data on the various causes of membrane durability.
- Technical progress includes both improved components and improved operating conditions to extend lifetime.
- Segmented cell testing in a stack is coming late in the program. Reduces opportunity for learning and feedback to MEA design.
- Durability prediction equation software has not succeeded in making independent predictions. It only seems to work if "tweaked" by actual testing results. This will limit usefulness of equation.
- Final system goals remain to be completed. Some doubt about this. Otherwise everything is proceeding well.
- There has been important progress but possibly less than would be expected relative to the time (3.5 years) and funding.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.4** for technology transfer and collaboration.

- Good within the "team".
- Would like to see more information disseminated outside the group.
- Strong collaborative team.
- Excellent collaboration with industrial research partner and 3 universities.
- Good team including analytical, supplier and OEM/system test partners.
- Good evidence that university modeling and testing was translated into MEA design and into system testing.
- Excellent.
- There is a good distribution of strong partners indicated, but it wasn't clear from the presentation that all are fully involved.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.7** for proposed future work.

- Program is ending.
- The proposed plan is adequate.
- The remaining portion of the project should focus on component improvements and completing the testing and post-test analysis, with lesser emphasis on modeling enhancement.
- Stack testing will proceed to failure.
- No clear plan for rectifying deficiencies in lifetime prediction modeling. If this only works when supported by test data, consideration should be given to stopping this effort now.
- No clear plan for integration of capillarity model into program goal of membrane durability.
- Incorporation of start/stop phenomena would make this more relevant to real world applicability. Constant power demonstration at system level is not realistic.
- Detailed future plans not given.
- There were no plans presented for efforts beyond the current contract (which is 90% done).

Strengths and weaknesses

Strengths
- Excellent team.
- Tied to all elements of a "stack" (suppliers, developers, end-users).
- Life-time prediction modeling.
- Long-term testing up to 8000 hours is an interesting feature.
- Stack validation was performed in a system.
- Nicely integrated contributions from university, component and OEM participants.
- Good empirical results.
- Very strong project.
- A strong team of researchers covering a wide range of capabilities. They have completed some important activities.

Weaknesses
- Too many team members.
- Not sure what the contributions were from each team member (based on the funding of each).
- Too many tasks.
- Tests were performed at steady-state conditions (shut-downs were once per month). More realistic cycling profiles are necessary. Correlations should be established between current distribution and cell degradation.
- Predictive equations still do not contribute much value.
- Some university contributions appear not to be fully integrated – why are they continuing?
- No weaknesses.
- It isn't clear that all team members have been fully involved.
- As it is currently formulated, the final results will have only limited usefulness.
- No follow up, with appropriate direction changes, seems to be even proposed.

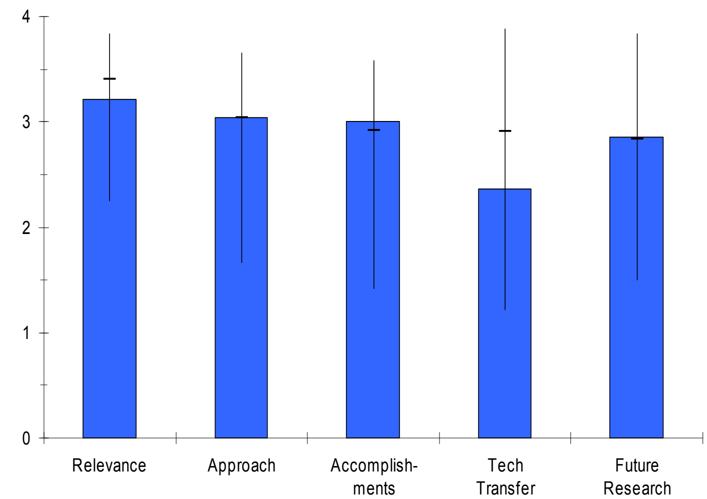
Specific recommendations and additions or deletions to the work scope

- Real life cycling tests are necessary (start/stop cycles).
- Need further project to develop in more detail the relationship of materials chemistry to failure modes and lifetime prediction.
- This project is near completion so it is too late for additions/deletions. However, a well-thought out (and redirected) follow-up program should be formulated and executed by a similar team.

Project # FC-11: Improved Membrane Materials for PEM Fuel Cell Applications
Robert Moore; U of So. Mississippi

Brief Summary of Project

Overall Project Score: 3.0 (7 Reviews Received)



The overall objective of this project is to ascertain and integrate critical structure-property information to develop methods that lead to significant improvements in the durability and performance of proton exchange membrane fuel cell (PEMFC) membrane materials. The specific objectives consist of 1) providing fundamental information regarding the origins of chemical and morphological degradation during accelerated chemical attack and PEMFC operation; 2) investigating the effect of modifications in membrane and membrane electrode assembly (MEA) processing parameters on performance and durability; 3) evaluating the role of controlled morphological features and reinforcing structures on membrane performance and durability; and 4) exploring the performance and durability of new hydrocarbon-based membrane materials as alternatives to the benchmark perfluorosulfonate ionomers. The objectives for FY 2007 for this project are investigations of membrane and MEA processing parameters on performance and chemical durability and the use of dielectric spectroscopy to probe molecular motions impacted by degradation.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.2** for its relevance to DOE objectives.

- Membrane durability and cost are key objectives of the Hydrogen Program.
- PI's project objectives are very well focused on providing an understanding of how morphological properties of membrane materials may be affected (improved/degraded) based on material processing and MEA fabrication conditions.
- It meets the DOE targets.
- In concept the project is relevant and can lead to a better understanding of the fundamental materials science of the key components of the MEA.
- Very relevant to commercialization of fuel cells with PFSA membranes for high temperature use.
- The work is generally relevant to the DOE effort to improve membrane durability and increase performance but the effort does not seem focused enough to result in a useful diagnostic by the end of the project.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- Need to demonstrate more clearly the relevance of the dielectric spectroscopy to the material properties and impact on Program and project objectives.
- Need to apply more diagnostics (e.g. conductivity measurement) to confirm and evaluate the changes that resulted from their annealing experiments.
- PI had clearly presented the connection between a material's morphological properties and fuel cell performance issues.

- Well organized approach, with initial emphasis on providing more (in-depth) insight for current membrane materials used today (and for the next 5-10 years), followed by a similar approach to examine new/alternative materials - relating physical properties to performance and durability.
- The presented methodology is satisfactory in meeting the objectives of the project.
- Approach is good as the techniques are useful in delineating elements of the fundamental polymer material science.
- The actual choice of materials, how they were processed and the tested could be re-evaluated to focus on membrane properties which relate to fuel cell conditions.
- Not sure the sol gel work should be part of this – focus on the polymer materials science!
- This has a very well thought out, systematic approach.
- The PI is a recognized expert in the field.
- Heat treatment studies on membrane are interesting and provide useful insight. Use of Si nanoparticles is poor idea. Si should never be added to any PEMFC membrane (hydration layer is small and it is highly soluble in acid environment).
- The approach is to develop methods to characterize the effects of degradation and to probe the origins of performance characteristics. There is some uncertainty regarding what actually is being studied by the dielectric spectroscopy (DS) method.
- The second approach is to modify Nafion membranes and MEAs by altering fabrication procedures, post-processing treatments, inorganic particle incorporation. The approach appears to be generally effective; however it is not clear how the knowledge gained in this study will be generally applicable to the community at large.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- The improvements in the polarization curve of the fuel cell with the annealed membrane are impressive, but also intriguing. The investigators should confirm with additional diagnostics.
- PI's accomplishments to date have included development of "screening tasks" needed for evaluating current and future membrane materials – and the relationship to fuel cell performance issues.
- The team appears to be meeting most of the current milestones.
- Accomplishments are just OK.
- There are many other questions and specific tests which should be performed and would be valuable in elucidating the polymer changes.
- The group must understand the membrane processing history as well, not just what they do to it.
- The assumption that melt-extruded film is the same as solution cast is not correct.
- Work describing changes in mechanical and chemical stability upon annealing is very good.
- This work provides a good, basic understanding of important properties of PFSAs.
- The results show that the acid form of the membrane degrades upon heating and becomes more susceptible to chemical attack. Fluoride release increases when the membrane is annealed above 200°C. This is not a favorable result.
- In the ionized form, the membrane appears not to degrade at elevated temperature.
- The DS technique can be used to characterize the relaxation of the polymer chains and determine the degree of shortening of the chains upon exposure to Fenton's reagent, potentially a valuable tool to determine the degree of degradation of a membrane.
- Hydrophilic silicate nanoparticles were incorporated into the polar domains of Nafion in the hope of creating hyperbranched structures with a large amount of open space and OH that will impart high-temperature water retention.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.4** for technology transfer and collaboration.

- There are no partners in the program. Membrane annealing results suggest they should have independent verification and further diagnostic application. Given they used NREL, why not DuPont?
- If the dielectric spectroscopy technique is indeed useful, there should be collaborations with other advanced membrane programs within the Program.
- PI and partner have consistently published their work, and routinely have made available their knowledge and expertise to others in the fuel cell program and industry.
- More links with other entities are needed.
- Acceptable.
- This project could benefit from collaboration with group with that can do more in-depth fuel cell evaluations.
- Collaborations need to be expanded especially in area of dielectric spectroscopy interpretation.
- The university is the only partner.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.9** for proposed future work.

- There's a lot of "Future Work" listed for only 6 months remaining in the program. Needs focus?
- Recommend they measure the conductivity of the annealed NRE membrane and attempt to understand what change actually occurred that increased the polarization curve performance.
- Recommend applying FC Tech Team durability protocols including RH cycling accelerated durability test.
- Future work plan is very aggressive for the May to November 2007 time frame.
- Examine whether thermal annealing is sustainable during operational conditions.
- Conductivity values after annealing should be measured.
- Focus on the polymer as opposed to trying to develop additives which are not new and which have not been shown to yield results yet.
- Expand the approach and testing as a function of the new materials being developed by 3M, DuPont etc.
- Focus on what the membrane "sees" during actual fuel cell tests.
- It will be interesting to see this work expanded to hydrocarbon systems.
- Inorganic additives need to be rethought and approach modified.
- Synthesis of hydrocarbon-based PEM membranes is only partially completed but was not discussed.

Strengths and weaknesses

Strengths
- Comprehensive approach, from material properties to fabrication requirements and how these two parameters affect fuel cell performance.
- Introduced broadband dielectric spectroscopy techniques for assessing membrane materials.
- Thermal annealing.
- The development of characterization methods to evaluate the effects of degradation is promising.
- Good team and good resources. Good use of an under-utilized technique.
- This work provides a good, basic understanding of important properties of PFSAs and addresses important issues in fuel cell commercialization.
- Fundamental membrane studies are relevant and provide insight and when coupled with inorganic additives should lead to improved membranes.
- The DS technique appears to be able to determine the extent of degradation of fuel cell membranes.

Weaknesses
- Impact of thermal annealing should be further investigated.
- Don't try to score a home run with respect to the additive task. Focus on what you know best – elucidate the polymer dynamics first.
- There is no consensus on the relevance of dielectric spectroscopy or how to interpret what the spectra mean. Some thought needs to be given to determine the relevance or moving on to other analytical techniques. Si should never be added to any PEMFC membrane (hydration layer is small and it is highly soluble in acid environment). Idea of inorganic additives good, but execution needs to be rethought.

- It is not clear that heat treating membranes will lead to improved durability or performance. More work is required to sort this out.

Specific recommendations and additions or deletions to the work scope

- The project scope may need to be re-assessed and reduced in scope, depending on the outcome of in progress investigations (i.e. "too successful").
- The project's duration (and funding) should be extended (increased) for the benefit of both industry and Hydrogen Program projects dependent on outputs from this project.
- Comparison of the current approach with existing results in literature should be performed.
- Ensure that the enhanced performance is not due to thickness reduction of the membrane.
- Add and enhance the tasks related to the techniques.
- It would be good to use gel permeation chromatography or another analytical technique to verify the theory that the MW is decreasing with degradation due to loss of small fragments.
- Add go/no go on dielectric spectroscopy.
- University of So. Mississippi should be encouraged to interact with membrane/MEA developers to explore the practical use and application of the DS technique.

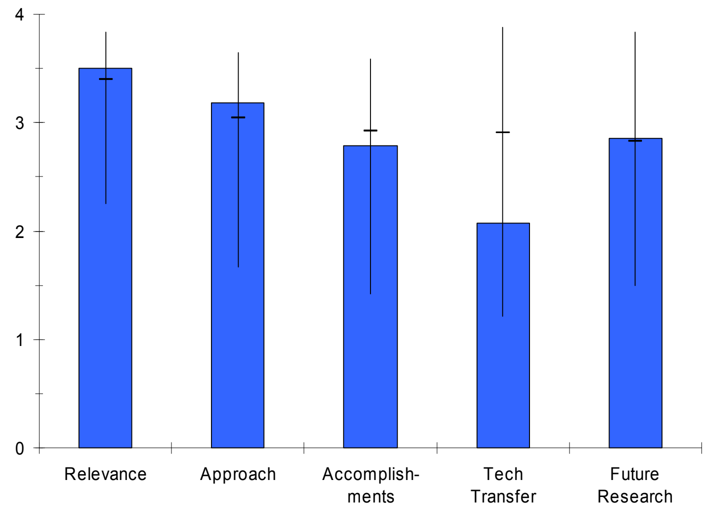
Project # FC-12: Poly(p-phenylene Sulfonic Acid)s with Frozen-in Free Volume for Use in High Temperature Fuel Cells

Morton Litt; Case Western Reserve University

Brief Summary of Project

The issues addressed in this project are 1) molecular weight; 2) graft copolymer synthesis; 3) conductivity; 4) permeability; 5) acid loss; and 6) oxidative stability. Polymer synthesis work for fiscal year 2007 has reproduced earlier results but with low molecular weight. Li salts were found to be soluble in N-methylpyrrolidone and dimethylformanide. The polymer trimethyl benzyl ammonium salt is insoluble in NMP. Grafting work for FY 2007 produced a successful reaction but the mechanical properties were too poor to cast films. Comonomer synthesis for FY 2007 consisted of grafting biphenyl in high yield using mild conditions but have not yet grafted t-butyl or neopentyl substituted aromatic moieties without some scrambling.

Overall Project Score: 2.9 (7 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

- The project is highly relevant to the DOE's objectives and to support the President's Hydrogen Fuel Initiative.
- Highly relevant to meeting DOE goals of enabling system simplification and cost reduction with low-RH membranes.
- Should be good means of introducing orthogonality to standard conductivity/solubility vs. EW trends.
- The target polymers intrinsically need water for conduction. This will require a large humidifier to maintain RH at 120°C. This does not address the long term problem. Is there any prospect of replacing water? The mechanism of water retention involves structures that limit the mechanical properties which will change with RH and temperature. This system is interesting scientifically but appears to lack robustness.
- Not entirely clear if these new types of membranes will meet cost targets (difficult synthesis with liquid crystalline polymers).
- Increasing operating temperature, especially for automotive application (cooling problems) and stationary application (CO poisoning), is addressed.
- Relevant.
- This work is highly relevant to the DOE technology goals. However, the goals were not clearly stated in the presentation and the presentation focused almost exclusively on the lower RH conductivity with dimensional stability, which is one key goal but other factors need to be considered and evaluated.

Question 2: Approach to performing the research and development

This project was rated **3.2** on its approach.

- The project is for 5 years. The project addresses polymer membrane electrolyte issue. The technical approach for the program is reasonable.
- Very interesting approach: creating structures that allow protonic transport even at lower relative humidities should allow for decoupling of equivalent weight and conductivity.
- Need to address solubility/decomposition in liquid water.

- The approach is sound. The investigator appears to have a good appreciation of the limitations inherent in the approach and is working around them.
- Other than the basic concept (e.g., copolymers with free volume), it is not clear what the approach is here.
- Good to start really at the basics for this new approach.
- Experienced, because of work done in 2002-2005.
- Through-plane conductivity should be reported especially if anisotropy is expected.
- Approach must be reevaluated if proper films cannot be formed.
- Nafion conductivity reported appears to be low . What temperature was it measured at?
- Agree with the general approach – novel polymers need to be developed. Believe this approach could be improved by defining progressive evaluation criteria beyond just *ex situ* RH/conductivity and dimensional stability. Recommend key project tasks should be stated and progress against such tasks highlighted (as in most other presentations)

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.8** based on accomplishments.

- The project was started April 2006. It is too early to make a judgment for technical accomplishments at this time. So far, the project progress is good.
- Impressive results on conductivity.
- Need to see more exploration of robustness in liquid-water conditions.
- Progress is good for a first year project due to prior work. Expect more progress in next year as staff becomes more familiar with the materials.
- Progress in the last year is not particularly impressive.
- Progress is slow, but that might be due to delayed start of the project.
- Important to overcome brittleness problem to get stable membranes.
- Project is at initial stage, thus, progress to date is modest. Only a single conductivity measurement is shown.
- Much of data shown were not part of this project.
- Problems to be addressed were well described from a polymer perspective.
- The tracking of progress against technical targets is challenging due to the focus on novel polymer development. Recommend a progressive evaluation of these materials against a set of *ex situ* and *in situ* goals. Interaction with other researchers/industry could be used to validate approach *in situ*.
- Delays in project start were described during the oral presentation which influenced and limited the progress made to date.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.1** for technology transfer and collaboration.

- The project was started April 2006. It is too early to transfer technology to industry.
- For early stages, measurement and testing in laboratory is appropriate, but as progress is made, need to engage outside partners for testing, processing, etc.
- No good connection to industry or an MEA fabricator. Need to consider this as an opportunity.
- Appears to be none, outside of Case Western Reserve University.
- Would be useful to involve industry partner, especially to look after cost and manufacturability.
- Unclear why only interactions with colleagues were reported.
- This was not highlighted in the presentation. Interaction with Samsung was mentioned.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.9** for proposed future work.

- Based on the presentation information, the future research work is clearly presented and technical approaches are reasonable.

- Needs a more concrete plan for next steps.
- Must address solubility issue.
- Further characterization of polymer in various states is needed.
- PI appears to be cognizant of pitfalls of approach, except for how to convert to completely water-free operation if water is not desired.
- The rationale for the next steps has not been well explained.
- Focus on just a couple of monomers/polymers should be done very early.
- This was not clearly addressed.
- No clear path forward observed.
- The proposed work is good; however it needs to include a wider set of goals with *in situ* criteria.

Strengths and weaknesses

Strengths
- The PI, co-Pi and coworker have excellent R&D experience for polymer membrane electrolyte and also for fuel cells.
- Very high conductivity at low RH.
- Unique approach.
- Good, experienced PI.
- Excellent fundamental understanding.
- The proposed work is good; however it needs to include a wider set of goals with *in situ* criteria. This project represents one of the most viable approaches of those reviewed.

Weaknesses
- Need to explain better how to address stability.
- Needs better tech transfer plan.
- Not clear where the engineering plays a role.
- How stable are these polymers? Does not appear to be much emphasis on determining stability under fuel cell conditions.
- No industry partner is involved.
- Materials studied appear to be ones with poor film forming ability measured Nafion® conductivity is very low.
- Very focused on novel material development without a fuller set of criteria for evaluation. No *in situ* evaluation in the plan.

Specific recommendations and additions or deletions to the work scope

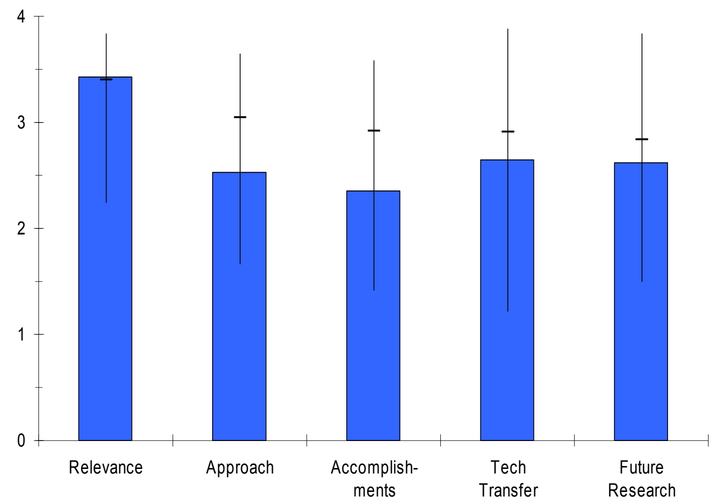
- This project just started the second year, project progress is good. No action is need at this time.
- Measure conductivity in the transverse direction. No good excuse for not doing this measurement.
- Involve industry partner to comment on manufacturability and cost.
- Measure through plane conductivity.
- It may not be productive to focus on materials that do not yield films.
- At a minimum, some degradation studies need to be performed on candidate materials.
- Collaboration with researchers/industry to evaluate more fully the materials developed.

Project # FC-13: Poly(cyclohexadiene)-Based Polymer Electrolyte Membranes for Fuel Cell Applications
Jimmy Mays; U of Tennessee

Brief Summary of Project

The objectives of this project are to synthesize and characterize novel neat and inorganically modified fuel cell membranes based on poly(1,3-cyclohexadiene). To achieve these objectives, a range of homopolymer and copolymer materials incorporating poly(cyclohexadiene) will be synthesized, derived and characterized. The successful completion of this project will result in the development of novel proton exchange membranes (PEMs) engineered to have high conductivity at elevated temperatures and low relative humidity.

Overall Project Score: 2.7 (7 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.4** for its relevance to DOE objectives.

- The pursuit of improved membranes for high temperature and low RH conductivity is reasonable.
- Polycyclohexadiene has not been studied as a polymer electrolyte and the ability to control polymerization in a living polymerization allows a phase space to be pursued that has not yet in polymer electrolytes.
- The oxidative and hydrolytical stability of the polymer has not been studied. The cross-linking sites and unaromatized rings are unlikely to have good chemical stability.
- Satisfies the DOE's request for a "fresh and novel" approach to identifying new materials for PEM membranes.
- Project is aimed at the discovery of new materials for PEMs that will operate under hotter and drier conditions.
- Project addresses important cost and durability issues.
- This work represents a new method of synthesizing sulfonated, crosslinked polyphenylenes. Such polymers may be useful in membranes, if conductive enough and stable enough.
- The project objective is critical for realizing renewable energy economy.

Question 2: Approach to performing the research and development

This project was rated **2.5** on its approach.

- The use of cross-links and post-sulfonation are both shortcomings of this proposal. Post-sulfonation gives poor control over location and extent of sulfonation. Cross-linking leaves weak chemical spots and increases brittleness.
- The characterization of the polymers has only focused on thermal properties; conductivity has not been pursued.
- There was no discussion about what block structures would be pursued or why they should be expected to yield better performance- this is particularly important in the context of post-sulfonation and crosslinking which could eliminate any of the advantages of a synthesized block.
- The premise for inorganic particle incorporation improving performance was loose and no results suggesting significant improvements possible were presented.
- Systematic, focused approach, coupled with excellent "Plan B" next step based on prior outcomes.
- This approach to reaching the DOE targets for higher temperature, drier operation is apparently new with the starting advantage of potentially very low cost materials.
- It is too early to anticipate where the major weaknesses of this approach will be, but some effort should be expended at the beginning to seriously identify the one or two major fundamental failure points that could prevent durability or conductivity performance targets from being achieved.

- Approach is solid and is focused on overcoming barriers.
- The stability of the cross-links is a concern, both the disulfide linkage and the aliphatic ring to which it is attached. It is not clear why these polymers would be superior to other sulfonated polyphenylenes or why this is the best method to prepare this type of polymer.
- The point of the sol gel aspect of the project needs to be made clearer. A lot of people have tried very similar things in the past.
- Clear strategy of obtaining high conductivity at low relative humidity is not laid out.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.4** based on accomplishments.

- While the project is rather new, far less data on these polymers were shown compared to other projects funded at the same time.
- Only a few polymers and membranes were characterized and the properties characterized were not the properties of primary concern for novel high temperature membranes.
- Excellent progress and very effective planning of experiments and related property analysis.
- Factual assessment of developmental materials, and if they meet targets.
- Films with good mechanical properties have been achieved.
- No conductivity data yet.
- The PI admits to a slow start.
- Good efforts to characterize the materials chemistry and structure.
- While it appears progress is being made with respect to cost reduction and material properties, clear status to targets should be shown.
- The researchers should measure the proton conductivity of these materials at this point to assess the viability of the approach. The durability should also be addressed soon, both *ex situ* (Fenton's tests) and in an MEA.
- The mechanical property testing is quite thorough.
- Successful synthesis of first trial of membrane has been accomplished.
- No activity has been shown on charactering key properties, conductivity and chemical and electrochemical stability.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.6** for technology transfer and collaboration.

- The combination of a characterization person and synthesis person makes good sense, however the type of characterizations performed are not those most relevant to the project, a person more familiar with electrochemical characterization may be a better choice. The techniques of Mauritz for evaluating polymer degradation are valuable, but not of primary importance for this project.
- Too early in program for technical transfer opportunities.
- Excellent use of University of S. Mississippi and ORNL to provide material property analysis, etc., and as a planning tool for determining the next steps in PI's program.
- Should consult with industry partner.
- Poor right now as it is a new idea just beginning in an academic laboratory.
- Consider expanding collaboration with membrane supplier.
- This program would benefit form collaborating with a "Fuel Cell" group (e.g., Los Alamos).
- Collaboration with institutes have capability of electrochemical property characterization is in need.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.6** for proposed future work.

- Future work on sol-gel chemistry leaves many questions about improvements possible.

- Brittleness as a primary problem suggests crosslinking is an issue, optimization of chemistry might be best served by looking at non-crosslinked samples as well.
- Cross-linking is a key issue, and the PI has assigned appropriate emphasis on this topic.
- Some comments on material manufacturing issues (barriers, etc.) would be a useful addition, once a candidate material has been identified.
- Improve mechanical properties.
- Incorporate sol-gel chemistry.
- Proton conductivity measurements.
- The project plans are very sensible for demonstrating progress toward the goals of improved conductivity.
- The PI should try to identify the most likely failure point of this technology and address it early – for example the susceptibility of hydrocarbon membranes to attack from peroxyl radicals.
- The use of Cl-containing crosslinking agents is a real concern, due to the potential for catalyst poisoning when the membrane is degraded by peroxyl radicals – it will happen. They should find alternatives.
- Project has several years to go, however future work is not described clearly.
- It is not clear what Type B or Type C polymers are, or how these would behave differently than the materials this group is currently studying. The conductivity has not even been measured on the current polymers.

Strengths and weaknesses

Strengths
- Novel materials with the ability to be made using living polymerization.
- Program well-defined and organized by the PI.
- Successful use of "experts" in material characterization to accelerate evaluation of candidate materials.
- Novel polymer architectures.
- Intelligent use of sol-gel chemistry.
- A new approach which always holds promise for new gains in performance.
- Strong collaborative effort with University of Southern Mississippi.
- The PI is working on the chemistry different enough to address the key issues, conductivity and cost of fuel cell membrane.
- Both groups present adequate experiences of developing new chemistry membranes for fuel cells.

Weaknesses
- Resulting structures to this point have not been characterized for conductivity. Chemistry being explored has significant chemical stability concerns. Crosslinking reduces processing possibilities and increases brittleness.
- All "high temperature, low RH" projects have a very high hurdle to achieve (e.g., conductivity).
- Fuel cell durability needs to be verified for "new materials", in addition to the conductivity target.
- PI can only post-sulfonate material. It is not clear that there will be any control of sulfonation chemistry.
- Cross-link chemistry illustrated in talk is totally unsuitable for fuel cell electrodes.
- No conductivity data.
- Combining the new polymer chemistry with the whole area of sol-gel chemistry is an enormous task to address for a level of this effort. The parameter space becomes enormous.
- The stability of the crosslinks is a concern, both the disulfide linkage and the aliphatic ring to which it is attached. It is not clear why these polymers would be superior to other sulfonated polyphenylenes or why this is the best method to prepare this type of polymer.
- The point of the sol-gel aspect of the project needs to be made clearer.
- No evidence has shown for the capability of characterizing electrochemical properties.

Specific recommendations and additions or deletions to the work scope

- Explore block chemistry further. Figure out what blocks may be possible and determine reasons why to pursue them. Specific recommendations would include developing monomers with protected sulfonic acid groups to avoid post-sulfonation or copolymerize monomers that don't allow random sulfonation.
- Reduce sol-gel chemistry effort.
- Eliminate cross-linking for at least baselining purposes.

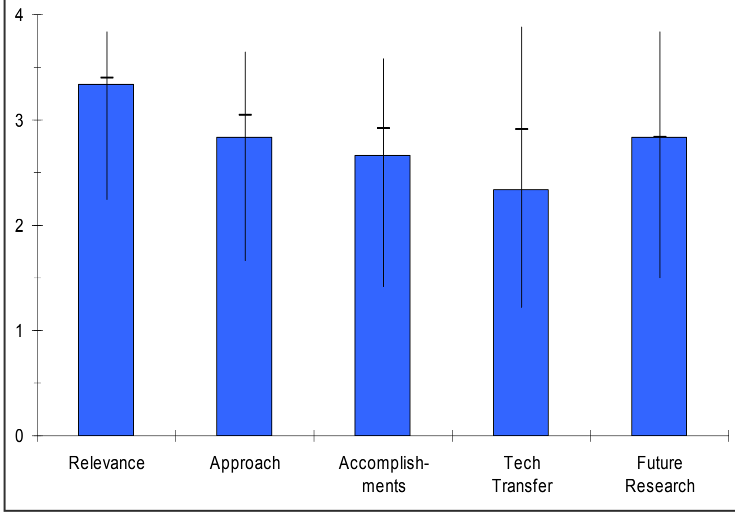
- The development of "new materials" may require additional technical resources (and funding).
- Find a fuel cell company or expert to consult with.
- Use proton conductivity for optimization; mechanicals can be improved after Go/No-Go decision is passed.
- Do some serious durability tests challenging the materials as soon as possible to get a feel for the baseline stability of the materials.
- Try to make full MEAs for fuel cell testing as soon as possible also, or better, work with experienced MEA testing group.
- When starting a new area, put some effort into trying to identify any fundamental failure mechanisms that will ultimately prevent success on that path, as well as developing all the good characteristics.
- Show status against DOE technical targets.
- The PI needs to put higher priority on characterizing electrochemical properties at the realistic operating conditions.

Project # FC-14: NanoCapillary Network Proton Conducting Membranes for High Temperature Hydrogen/Air Fuel Cells
Peter Pintauro; Case Western Reserve University

Brief Summary of Project

The objective of this project is to fabricate and characterize a new class of NanoCapillary Network (NCN) proton conducting membranes for hydrogen/air fuel cells that operate under high temperature, low humidity conditions. To achieve these objectives, the project will employ electrospun nm-sized fibers of a high ion-exchange capacity polymer that are vapor-welded and imbedded in an uncharged polymer matrix. There will be an addition of molecular silica to further enhance water retention. Additionally, the project will employ the concept of capillary condensation for membrane water retention.

Overall Project Score: 2.8 (6 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

- High temperature membranes are critical to the realization of the Hydrogen Fuel Initiative, to increase system performance and efficiency and to reduce system cost and volume to meet automotive targets.
- Membrane material test conditions should mimic real world usage profile and temperature and humidity should be defined. For automotive applications, a wide range of temperature and humidity (hydration) should be tested. High temperature operation is very small fraction of entire life (less than 5%).
- Relevant.
- This project has highly relevant technical goals towards the DOE technical targets for this critical core component.
- The project objective is critical for realizing renewable energy economy.

Question 2: Approach to performing the research and development

This project was rated **2.8** on its approach.

- Good approach to membrane morphology (NCN structure).
- Novel approach to membrane fabrication.
- Silica has limitations.
- Unique approach, however, is this cost effective compared with conventional membrane process?
- Materials stability of additives, water retention, in the membrane under condition (hydration) changes.
- Fuel cell test will be necessary to validate membrane structure optimization.
- Approach is novel, but lacking focus.
- Chemical production not considered.
- The technical approach presented is logical and appropriate.
- Identifying the desired pore structure for water retention and conductivity can help to expedite the development.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.7** based on accomplishments.

- Membrane fabrication process demonstrated and optimization initiated.
- Treatments of material show promise to increase conductivity.
- Membrane conductivity at high temperature and low RH not investigated yet.
- Too early to discuss technical outcomes. Performance is still low.
- Lacking relevant fuel cell results.
- Good proof of concept.
- Unclear how low RH conductivity target can be met.
- Given the limited effort thus far, this project has made excellent progress.
- Demonstrated the feasibility of making capillary network membrane using electrospinning.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.3** for technology transfer and collaboration.

- Collaboration with Wright State University for polymer synthesis seems to have yielded polymers suitable for electrospinning.
- Polymers with higher conductivity have been prepared.
- Fuel cell testing will be necessary for membrane material/structure optimization and this could be a collaboration opportunity.
- Could use cross fertilization with other fuel cell experts at Case.
- Good team.
- As this project is in its initial stages, the amount of collaboration is appropriate.
- Contributions from the partners are not discussed.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.8** for proposed future work.

- Logical plan focuses on opportunities to increase conductivity and improve the membrane properties.
- Plan for molecular silica is not clear.
- Materials stability should be evaluated, e.g., water retention of additives.
- Electrode interface characteristics should be investigated prior to fuel cell testing.
- Gas separation should be evaluated (hydrogen permeability).
- Need to add some basic fuel cell test to demonstrate viability of approach as well as water uptake and stability tests. More detailed approach is needed.
- Low RH studies must be done → not claimed. Otherwise very comprehensive.
- The proposed project work is appropriate, given the early stage of this exploratory work.

Strengths and weaknesses

Strengths
- Novel approach.
- Membrane material/membrane process.
- Membrane performance testing.
- Novel concept.
- Very experienced P.I.s.
- Proof-of-concept very convincing.
- This project investigates a potentially viable PEM membrane structure which may address one of the failure modes of dense PEM membranes.
- Significant progress has been made.

Weaknesses
- Membrane tortuosity and durability are of concern.

- Understanding of application and usage conditions.
- This project lacks cohesion and a proper set of detailed tests to determine uptake and stability. Approach needs validation. At present, approach would appear to increase proton path length which would decrease power. PI needs to prove this concept.
- Low RH conductivity will be an issue with material used.
- High temperature stability of thermoset is questionable.
- There is no theoretical investigation for the structure of the membrane to quantify the required properties of water retention.

Specific recommendations and additions or deletions to the work scope

- Recommend confirmation of the basic requirement of PEMs for fuel cells, gas separation is one of the critical requirements. Need to clarify how this porous membrane achieves enough gas separation.
- Need to estimate ball park cost to identify cost benefit compared to conventional membrane process, e.g., casting.
- There should be a go/no go decision gate added in the program plan (if it isn't there already) to evaluate the feasibility of the electrospun, PEM fiber matrix approach to achieve the required membrane conductivity.
- Recommend a cost assessment of this approach be included in the project objectives to ensure these additional manufacturing steps do not add excessive cost.
- Recommend rework on project plan, including definition of basic requirement of PEMs for fuel cells and technical problem to be solved in this project.
- Set proper performance evaluation items with respect to defined basic requirement.
- Confirm the structure and materials are within reasonable cost to make a fuel cell. Ball park cost estimation is recommended.
- Detailed study of active fiber loading in an inert matrix to determine conductivity, power, uptake and stability.
- Durability studies to be added (chemicals).
- Low RH studies to be added.
- Addition of a go/no-go decision gate to assess the viability of the electrospun, matrix approach to achieve the DOE proton conductivity targets without losing the functional advantages of the impregnated matrix.
- Possibly include collaboration with others to examine alternative polymer electrolyte materials for the electrospun matrix approach.
- The PI needs to quantify the desired property/structure for water retention.

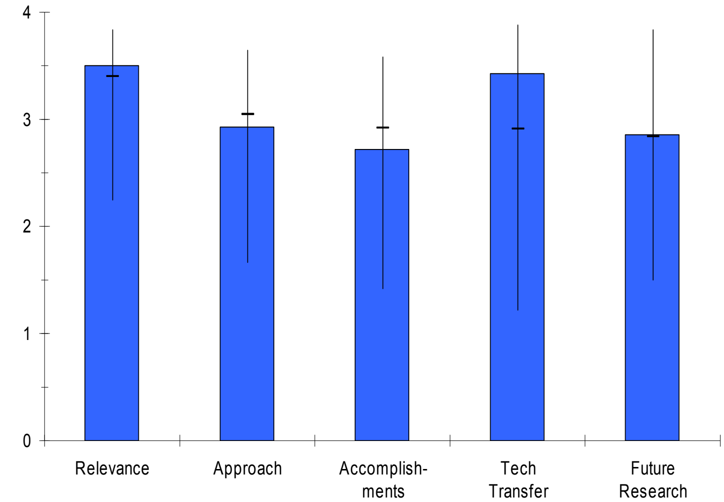
Project # FC-15: Lead Research and Development Activity for High Temperature, Low Relative Humidity Membrane Program

James Fenton; U of Central Florida

Brief Summary of Project

The objectives of this project are to 1) employ new polymeric electrolyte/phosphotungstic acid membranes; 2) standardize characterization methodologies (conductivity, mechanical, mass transport, and surface properties, durability); 3) provide High Temperature Membrane Working Group (HTMWG) members with standardized tests and methodologies (short courses); and 4) organize HTMWG bi-annual meetings. Task 1 membranes use non-Nafion based poly[perfluorosulfonic acid] – phosphotungstic acid membranes and membrane electrode assemblies (MEAs). Task 2 membranes use sulfonated poly(ether ketone ketone) or sulfonated poly(ether ether ketone) – phosphotungstic acid composite membranes and MEAs.

Overall Project Score: 3.0 (7 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

- The development of high temperature/low RH membrane materials is highly needed for the successful commercialization of PEMFCs.
- Standard of proton conductivity in-plane and through-plane testing is very important for the industry.
- The coordination of the HTMWG is a significant responsibility, although the separation of this as a research project and a coordination project make its review more difficult.
- The use of HPAs with Nafion or PEEK is not novel; using lower EW materials make sense for conductivity reasons, but leaves big questions regarding stability.
- Coordination of HTMWG is valuable work.
- The development of a high temperature, low relative humidity proton-conducting membrane electrolyte would reduce system complexity and cost and enable the application of this technology to automotive propulsion power.
- PI has identified reasonable alternative membrane materials and additives to meet the project's objectives.
- PI had made concerted effort to assist other project PIs in evaluating their choice of alternative materials, which will benefit all DOE projects in this area.
- The activities are clearly relevant. However, there are some holes that are worrying. There appears to be no provision for mechanical properties and gas permeation.
- This is a critical activity to identifying new membranes which will meet DOE targets.

Question 2: Approach to performing the research and development

This project was rated **2.9** on its approach.

- Immobilized PTA in PFSA materials could help with low RH performance but it is unclear how mechanical improvements can be achieved.
- sPEKK and sPEEK are notoriously brittle. While low RH performance with immobilized PTA could be beneficial, it is unclear how mechanical improvements can be achieved also with this material system.

- Proton conductivity work is very important and being pursued in an excellent manner.
- The significant effort being used to baseline conductivity measurements is reasonable as these are the primary properties of concern. Addressing water uptake would also be useful.
- In-plane conductivity seems reasonable for almost all samples tested; some question exists about how much effort should be expended on through-plane measurements.
- Addition of PTA not expected to enable achievement of membrane performance goals.
- Effort to standardize conductivity measurements for all HTMWG programs is good approach.
- The coordination and lead laboratory aspect of this project is excellent.
- The approach to standardizing testing and reconciling some of the differences in various testing protocols is outstanding and the results will be invaluable.
- The approach to developing new materials is not novel and it is unclear what new aspect these PIs bring to this approach.
- Well-organized and focused on two main objectives: development of new membrane material and reliable conductivity measurement instrumentation.
- Good approach (material and additive selection) for achieving conductivity at both high and low RH.
- Approach is good for the organization of the measurements. However, the lack of polymer mechanical characterization and how mechanicals help in making electrodes and MEAs is critical. This is missing and must be rectified.
- More focus should be put on working with other 11 group members. Each material will have different needs for adequate testing and evaluation. It is important that this not be just "screening".

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.7** based on accomplishments.

- PTA/PFSA materials show promising proton conductivity results.
- PTA/HC materials show very low PC; not clear how the PI will level up the data.
- In-plane/through-plane conductivity is progressing very well.
- The project is rather new, and has thus far focused on baselining efforts; while these are reasonable they don't advance towards lower RH conducting membranes.
- Results shown for Nafion composites don't look that different from IONOMEM results, and no strong reason for expected improvements in conductivity using PEEK was presented.
- Significant work has been accomplished in automating data on conductivity as a function of RH.
- Showed progress in in-plane conductivity testing at Bekktech.
- PI successfully made numerous polyelectrolyte membranes with PTA, but data shows no significant performance benefit.
- This team has made excellent progress in baseline proton conductivity measurements of Nafion membranes.
- Initial material development efforts are on target and well documented.
- Development and qualification of conductivity instrumentation on target.
- So far so good, but add the dimension of polymer mechanical properties.
- It should be shown how "characterize mechanical, mass transport and surface properties of membranes" and "predict durability of membranes and MEAs fabricated from other eleven HT low RH membrane projects" will be carried out.
- A very good system of conductivity evaluation has been put together. These measurements can be quite difficult.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.4** for technology transfer and collaboration.

- Good collaboration with BekkTech.
- HTMWG may want to implement industry more to get a realistic perspective on membrane needs.
- The combination of people in this project makes sense for the oversight part of the project. The only question being the appropriate level of effort for through-plane conductivity.

- The development of novel materials seems to be an independent endeavor.
- Strong collaboration with BekkTech & Scribner for conductivity testing.
- PI organizes HTMWG meetings with all other PIs.
- By definition, the category two winner must have well-established collaborations and transfer of technology. It is apparent that this aspect of the project is working very well.
- Collaboration with commercial membrane and MEA manufacturers would ensure the timely transfer of newly-developed membrane technology to the application.
- PI has made excellent progress in coordinating the qualification of both in-plane and through-plane conductivity measurement instrumentation and protocols with external consultants and commercial suppliers.
- PI's "extra efforts" to hold workshops for university and national lab participants in the High Temp/Low RH program, and offer to test their "in-progress" material development efforts prior to the "go/no-go" deadline.
- Good.
- The High Temperature Membrane Working Group has an excellent group of researchers.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.9** for proposed future work.

- Continuation of PTA/PFSA material is worthwhile – unclear how worthwhile the PTA/HC materials are considering how far they currently are from the DOE Go/No-Go targets.
- Proton conductivity continuation is important and being finalized.
- Future work is reasonable, but is unlikely by itself to contribute significantly to obtaining materials with the requisite properties.
- Developing standard through-plane conductivity test is a good idea.
- PI plans to evaluate lower EW membranes with HPAs.
- No durability test plans specified.
- Continued work on through-plane conductivity measurements is outstanding.
- Very little detail was given on the direction of the research in new membrane development.
- PI's plans for low EW ionomers and new formulations of sPEEK, sPEKK, etc. may need concurrent durability analysis in addition to the "conductivity" goal.
- Too little information was provided. There is no discussion of starting any fuel cell testing, mechanical property testing, or anything other than conductivity testing. These activities are critical.

Strengths and weaknesses

Strengths
- Excellent project management.
- Excellent partners of BekkTech and Scribner.
- It appears an automated and efficient process will result in meeting key deliverables.
- Leadership of HTMWG.
- Knowledge and coordination skills of the PI.
- Focus on standardization of testing procedures.
- Development of reliable conductivity instrumentation vital to all high temperature/low RH membrane participants.
- Novel approach to incorporate PTA for improved conductivity.
- Excellent start on conductivity testing.

Weaknesses
- Material novelty and potential seems to be rather weak – should step out of the box a little more.
- New materials development doesn't show particular insight and is unlikely to lead to further improvements necessary to reach DOE goals.
- Approach of adding PTA to existing sulfonic acid ionomers not likely to meet DOE high temperature performance targets.
- No focus on durability.

- Lack of rationale for the use of phosphotungstic acids.
- Lack of high-temperature, low relative humidity conductivity data for newly-developed membranes here and for all high temperature/low RH membrane projects – it may be very difficult to achieve the conductivity target.
- Polymer mechanical properties are missing.
- It is not clear to what extent the project leading and coordinating the High Temperature Membrane Working Group as a fuel cell membrane testing expert, and to what extent it is to use the polymers developed by the group to develop a new phosphotungstic acid doped membrane. I'm not sure these goals are compatible within the same program.

Specific recommendations and additions or deletions to the work scope

- Continue to work on project management and proton conductivity.
- Unclear what the PTA composite membranes are bringing to the fuel cell community – does the PI really think this material can be commercialized and implemented in a vehicle?
- Delineate the project better between a research project and an administration project.
- PI should run durability tests on membranes with and without PTA.
- HTMWG meetings should have more technical content & discussions.
- HTMWG should focus more on durability.
- May be appropriate to set up a "support lab" for conductivity measurements, since not every project PI will be able to install the instrumentation. In the future, this might be a suitable project for a national lab (ORNL, etc.), or turn over to industry (service work and/or instrument supplier).
- Add a polymer specialist to the team.

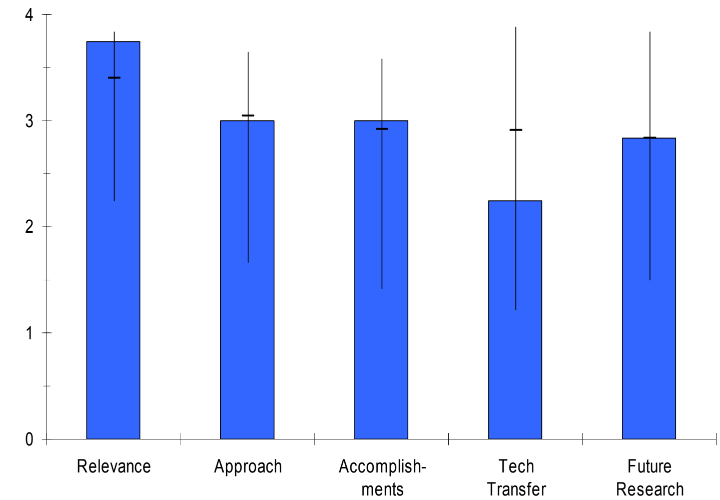
Project # FC-16: Protic Salt Polymer Membranes: High-Temperature Water-Free Proton-Conducting Membranes

Dominic Gervasio; Arizona State

Brief Summary of Project

The objective of this project is to make proton-conducting solid polymer electrolyte membrane (PEM) materials. These PEM materials should have 1) high proton conductance at high temperature (up to 120°C); 2) effectively no co-transport of molecular species with proton; 3) reduction of fuel cell overpotential; and 4) good mechanical strength and chemical stability. Protic ionic liquids (PILs) will be used to model membranes. Acid and base moieties and polymer properties will be varied to optimize properties of the protic salt membrane. The first goals are to make a stable liquid then membrane electrolytes with a conductivity >0.2 S/cm at 120°C and >0.0005 S/cm at -20°C.

Overall Project Score: 3.0 (6 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.8** for its relevance to DOE objectives.

- Project focuses on the development of high-temperature, low-humidity membranes using protic ionic liquids.
- Clearly addresses DOE targets and goals.
- High performance membranes capable of operation at high (up to 120°C) temperature are a key objective of the program.
- Aligned with DOE goals for PEM membranes.
- This pursuit of a new electrolyte provides a possible alternative to existing technology and may lower costs and may improve performance.
- Alternative electrolytes may provide a pathway to increase commercialization.
- Solid electrolytes could bring benefits of durability, higher proton conductivity, and lower cost.
- The objectives of this project are fully aligned and highly relevant to the DOE technical goals.
- This project is a higher risk, fundamental materials study which addresses in novel ways the DOE technical goals.
- The project objective is critical for realizing renewable energy economy.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- Good task description; well thought out.
- Approach addresses identified technical barriers.
- Approach (protic salts) appears novel and at least has some promise (high temperature, non-aqueous, high performance shown at very low current density) of achieving 120°C target.
- Addresses technical barriers for conductivity at very low-RH and high temperatures.
- Conduction mechanism is not dependent on the presence of water.
- While work with ionic liquids in porous matrices and sorbed in polymers will help develop this class of fuel cells, for an automotive membrane, need to focus more on immobilized PIL concepts.

- This approach is starting from a position that is less advanced or developed than others, but has a higher potential payoff.
- The program plan effectively addresses the issues in a methodical manner.
- The methods used – moving from liquids to solids – was chosen to improve the likelihood of success.
- The transition from liquid to solid is one difficult hurdle – this may make the chosen method more difficult.
- The approach described is logical and addresses the appropriate technical barriers in an appropriate order.
- The PI needs to identify the strategy of obtaining both stability and conductivity.
- Morphology studies of stable protic salt membranes are needed.
- The project unitizes a new water-free conduction approach.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- Given the project is only 20% complete, progress to date has been good. Several membranes incorporating protic ionic liquids (PILs) have been synthesized and initial testing complete.
- Initial results are encouraging.
- While a long way to go from liquid salts to a membrane, progress appears more than commensurate with the elapsed duration of the program.
- Some promising conductivities. But need to combine with stability and performance at higher current density.
- Demonstrated fuel cells with liquid protic ionic liquids with some advantages.
- Conductivities need to be improved, especially for non-leachable systems (need orders of magnitude improvement).
- The progress, compared to the total project timeline, appears to be tracking well.
- The accomplishments so far appear to be tracking towards resolution.
- It seems to be too early to make a final judgment, but progress so far is good.
- Investigations into mechanisms of proton transport are very good and appropriate.
- Understanding of stability mechanisms is an important factor that requires characterization.
- Demonstrated the feasibility of making protic salt membrane electrolytes.
- The limiting step of the proton conduction needs to be identified to address the conductivity issues with stable membranes.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.3** for technology transfer and collaboration.

- Reference made to Boeing collaboration but actual interaction was not documented.
- Collaborations are unclear.
- Collaborations with other universities.
- Not clear what Boeing's role is.
- The project includes collaborators, but little collaboration was mentioned outside the project participants.
- Some additional technology transfer, perhaps to the SECA program, might be beneficial.
- Given the initial phase of research, collaboration with researchers in other specialities has been appropriate and results are encouraging.
- Contributions from the partners are not discussed.
- Collaborations for morphology characterization of the membranes are needed.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.8** for proposed future work.

- Future plans are adequate and directed toward achieving DOE targets.
- Concentrate on developing and characterizing conductive, durable (non-leaching, non-dissolving) PIMs before rushing to the next level (i.e., fuel cell testing).

- Work with ionic liquid filled PEMs will help understanding of these materials and fuel cells based on them but immobilized PILs are what is applicable to the high temperature membrane project goals.
- NMR experiments should be helpful in determining proton transport properties and mechanisms.
- The project is early in its timeline. Future work is the majority of the work.
- Proposed future work seems consistent with the overall project plan.
- Project is progressing well and future research is appropriate and well considered.
- Consideration of potential issues with developing electrode needs to be planned.

Strengths and weaknesses

Strengths
- PI seems knowledgeable and well-qualified to perform the proposed research.
- Novel approach that, in theory, has promise.
- Concept with the potential for a truly non-aqueous conduction mechanism.
- Solid PEM electrolytes are a unique field, providing much opportunity for innovation.
- Project plan appears to be logical – moving from liquid to solids.
- Project has achieved much in a short period of time.
- Good exploratory work into novel materials.
- The project utilizes a new water-free proton conduction mechanism for novel membrane development.

Weaknesses
- Membrane stability and catalyst poisoning may be issues in the future affecting fuel cell performance and durability.
- It may not be possible to find a viable solid electrolyte to meet the goals. Many barriers remain.
- Some lessons learned from other technologies (e.g., SOFC) might be helpful, but have not been discussed.
- The project has insufficient planning and collaborations lacking morphology and electrochemical aspects.

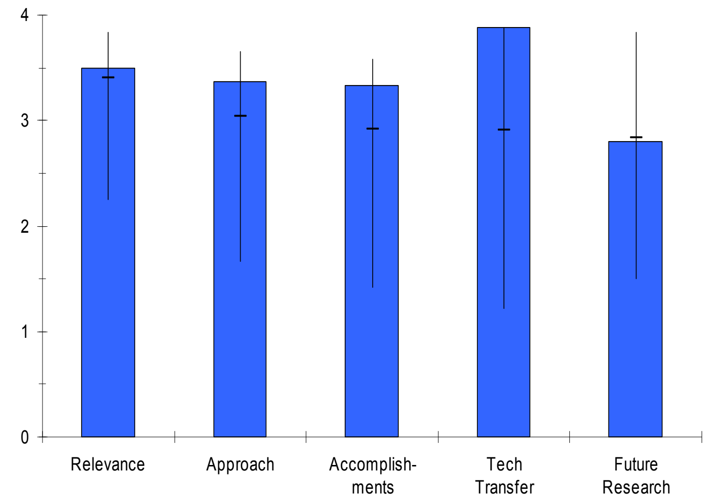
Specific recommendations and additions or deletions to the work scope

- Work with experienced MEA developer to allow program focus on electrolyte.
- It is too early to recommend changes at this time. The project is progressing well.
- Addition – evaluation of these PIL materials as catalyst ionomers (this was implied in the presentation but could be added to the project objectives). If this could reduce the cathode overpotential loss, this might be advantageous for all fuel cell applications.
- Morphology studies are in needs for the stable protic salt membranes.

Project # FC-17: Novel Approaches to Immobilized Heteropoly Acid (HPA) Systems for High Temperature, Low Relative Humidity Polymer-Type Membranes

Andrew Herring; Colorado School of Mines

Overall Project Score: 3.3 (6 Reviews Received)



Brief Summary of Project

The overall objective of this project is to fabricate a hybrid HPA polymer (polyPOM) from HPA functionalized monomers with $\sigma > 0.1$ S cm^{-1} at 120°C and < 1.5 kPa H_2O. The objective for fiscal year 2007 was the synthesis and optimization of hybrid HPA polymers for conductivity from room temperature to 120°C. Phenyl HPA derivatives will be subjected to low pH/ high temperatures to determine optimum chemistry for fuel cell stability. A determination will be made of the most facile conversion of HPA polymers to proton conducting systems.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

- The development of high temperature/low RH membrane materials is highly needed for the successful commercialization of PEMFCs.
- The need for increased membrane performance at low RH exists, but it is not the primary barrier to commercialization.
- Objectives are addressed by program elements.
- Concern with proprietary efforts around material supply and "smart formulation" for film formation.
- Development of membranes for low humidity and high temperatures is one of the key issues for DOE.

Question 2: Approach to performing the research and development

This project was rated **3.4** on its approach.

- Immobilization of "polyPOM" in polymer materials is very important for the success of this program and is being pursued by the PI.
- Use of caustic pre-screening of cross-linker is an excellent way to speed up development time and prevent dead-ends.
- Inorganic heteropolyacids have shown promise for high temperature fuel cell use; few others are modifying chemistry and directly incorporating into polymers the same way as this group.
- Novel approach (HPA moieties), and "new territory".
- Consideration of hybrid organic-inorganic monomer HPAs.
- Unique approach that appears to hold promise.
- Good approach to start at the basic monomer work and going then step-by-step up to membrane stability at 120°C.
- The approach recognizes previous work done with heteropoly acids and builds on previous work.
- CSM recognizes risks related to oxidative stability and taking a success-oriented approach. Oxidative stability may have to be addressed later.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.3** based on accomplishments.

- "polyPOM" relies on water for proton conductivity – unclear how proton conductivity at low RH is possible when "polyPOM" is blended with polymer "X". No data was shared to prove this concept.
- Focusing on linkages that survived caustic tests is a very good idea.
- 100 plus films to date is significant and must be leveraging other work.
- Reported performance for compounds besides the pure powders is still very low.
- The proprietary nature of some of the data makes it difficult to technically review.
- Reported progress is satisfactory.
- Program may require additional personnel, since initial results indicate the program may require additional effort to assess and resolve "new issues", similar to those reported (stability of initial candidates).
- Appears to be good results for this point in the program.
- Fundamental understanding of phosphate linkage and model phenyl derivates.
- On-schedule achievement of the first project milestone appears likely.
- The project is fairly new but important progress has already been made.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.9** for technology transfer and collaboration.

- Collaboration with 3M provides the needed guidance to the PI on this novel concept.
- Collaboration with 3M is extremely valuable as they can potentially help commercialize.
- PI's project will benefit from identified industrial partner (3M), who can provide the necessary materials, processing and fabrication support for this program.
- Good collaboration between institute and their "friends" from 3M.
- Collaboration with 3M Company is advantageous and has facilitated progress.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.8** for proposed future work.

- Incorporation of "polyPOM" in polymer "X" with significant testing of membrane properties is very important and scheduled.
- Methacrylate-based systems may not be the best choice for durability.
- Project should place more emphasis on oxidative stability of polyPOMs.
- Good plan to elucidate understanding, as well as drive towards a viable material.
- Focusing also on MEA preparation and test. The best membrane is nothing when it does not work together with the electrodes.
- No obvious show-stoppers have been identified although a few significant technical hurdles are listed.
- Critical involvement of 3M for the next steps is recognized by CSM.

Strengths and weaknesses

Strengths

- Novel concept with high potential.
- 3M's ability to keep the PI focused on the application.
- Good team, novel area of pursuit.
- Alignment with 3M for polymer synthesis and polymer conversion to membrane.
- PI appears to be well aware of what the targets are for membranes (e.g., good conductivity at 120 and -20°C with little water).
- Partnered with 3M early to help ensure that membrane is commercially viable.
- Good understanding due to having and testing model systems.

Weaknesses

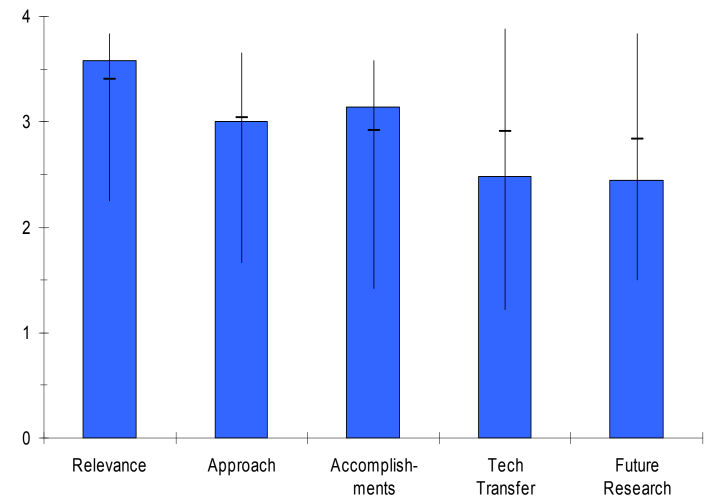
- Unclear how polymer "X" will provide the ability to conduct protons at low RH. No proof of concept was shown due to IP issues.
- Based on the data presented (and no other clear rationale for significantly improved performance), it seems unlikely that these materials can be improved enough to meet DOE targets.
- Conversion of HPA to free-acid may be a challenge.
- Polymer durability in fuel cell environment needs to be actively addressed.
- PI not able to discuss actual formulations.
- CSM is deliberately delaying addressing some technical hurdles that may turn out to be show-stoppers (3rd bullet slide 23).

Specific recommendations and additions or deletions to the work scope

- The program thus far is on track.
- Upon blending with polymer "X", significant testing will be necessary to prove this particular concept for the "Go/No-Go" decision.
- Need to create a compelling story for what level of conductivity these types of materials can obtain.
- Continued/additional emphasis on low RH conductivity (< 70% RH).
- Add work on MEA.

Project # FC-18: High Temperature Membrane with Humidification-Independent Cluster Structure
Ludwig Lipp; FuelCell Energy, Inc.

Overall Project Score: 3.0 (5 Reviews Received)



Brief Summary of Project

The technical accomplishments of this project were: 1) a multi-component composite (mC2) membrane concept was defined; 2) an improved baseline polymer was selected and characterized (6 month milestone met); 3) additives for water retention and protonic conductivity enhancement have been identified and fabricated; 4) measurements were verified by BekkTech; and 5) conductivity is used as a "figure of merit" and mechanical properties were used as a check point.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.6** for its relevance to DOE objectives.

- The development of a proton-conducting membrane that can operate under low relative humidity conditions and high temperatures will enable the widespread implementation of this technology to solving the country's energy needs.
- The project supports the overall DOE objectives, and if successful, could simplify fuel cell system requirements and thereby reduce overall fuel cell system costs.
- A new electrolyte provides a possible alternative to existing technology, may lower costs and improve performance.
- Alternative electrolytes may provide a pathway to commercialization.
- The focus on the target of high temperature membranes is appropriate.
- The materials are clearly being fabricated to meet the automotive DOE conductivity/area resistance targets for room temperature and 120°C.
- There is no indication as of yet that any of the DOE targets for membranes are being ignored.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- Approach is good as it combines aspects of many other successful approaches, however, it is difficult to fully evaluate the approach without the identity of the materials.
- The baseline polymer shows conductivities far from the DOE 2010 target – what is limiting this conductivity?
- The project approach, based on a multi-component composite membrane concept, is technically sound.
- Project plan is methodical and planned to move from material to material – this is a strength.
- Project builds upon success, using additives to increase performance – this is a strength.
- The approach is rather "standard", that is a new membrane with additives. There was not enough information about the materials presented to evaluate the novelty or merit of the approach adequately.
- Approach to addressing conductivity, water retention, and mechanical support is clear.
- "Stabilized nano-additives" are described as the approach to maintaining conductivity at freeze conditions. These nano-additives are either not mentioned in the drawing showing the membrane concept, or they are confounded with some of the other additives.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.1** based on accomplishments.

- Good progress in establishing a baseline polymer with improved conductivity compared to Nafion.
- Without the identity of the baseline polymer or the mechanism by which it achieves its improved performance compared to Nafion, it is difficult to evaluate if this baseline polymer is a viable candidate for long-term operation in the fuel cell.
- Good technical progress achieved so far in very little time (9 months) with low level of effort (<$250K).
- Shown conductivity of 2.5 x Nafion – good result.
- Conductivity tracks Nafion over the range of RH – good result.
- Additive studies show opportunity for improvement.
- Worked hard to obtain good repeatable data – shows rigorous scientific application.
- Checked data against an independent testing lab – good approach.
- The additives described seem to be quite effective. Also the extruded, baseline membrane seemed to have very good conductivity.
- The speaker said that the additives had the same relative effect on the newer extruded membrane as they had on the cast membrane (data in slide 11). Additive B seemed to provide an increase in conductivity at 30 % RH of about 5 to 6 x. If that is the case, the additive would raise the conductivity of the baseline membrane to 100 mS/cm at 120°C, 30% RH. Is this the case?? These conductivity values should be reexamined.
- The extruded baseline polymer is far from the DOE target at 120°C, although progress has been made from the original cast material (6 to 30 mS/cm at 40% RH).
- Verbally, it was stated that the water retention and conductivity enhancement additives will provide the same benefits for the extruded material that they did for the cast material. These data need to be shown.
- Mechanical stability should be shown with an *in situ* test such as an extended mechanical cycling test (quick cycles of 100% RH and dry gas).
- Low thickness shown (25 μ).

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.5** for technology transfer and collaboration.

- No partners in this project. Only apparent outside interaction is with BekkTech for conductivity tests.
- Good participation with other researcher on developing testing protocols, and independent measurement of membrane conductivity.
- Collaboration with testing laboratory is laudable.
- The team includes diverse collaborators, including potential customers – this is a strength.
- The close work with UCF and Bekktech is an important aspect of this program to allow good evaluation of these new materials.
- Collaborators listed are expected within the context of DOE high temperature projects (DOE, BekkTech, UCF).
- Although it is difficult to suggest collaboration at present, it is expected that project hurdles will necessitate collaboration. For example, the mechanical support may be addressed, but what if an additive is unstable or leaches? Are there large membrane producers that have experience with additives that could be of assistance? How much experience does FuelCell Energy have with adding additives to membranes?

Question 5: Approach to and relevance of proposed future research

This project was rated **2.4** for proposed future work.

- No details were given as to what would be done in the future research beyond "improve materials and processes".
- Work plan for future development is clearly defined and well structured.
- Project is early in its schedule. Future work is consistent with project plans.

- More information should be provided. The proposed future research seems to be to "optimize the membrane and meet the targets".
- Achieving only the room temperature conductivity target by next year is not aggressive enough.
- It is not understood what is meant by "improve functionality of individual components." Does something have to be improved regarding the individual additives before they can be fabricated into the membrane?

Strengths and weaknesses

Strengths
- Multi-pronged approach to achieving DOE membrane targets.
- Alternative electrolytes are a field with many opportunities.
- The project plan appears to be well thought-out and methodical.
- Verification of project data by a third-party laboratory helped to validate the data protocols – good practice.
- Excellent results so far.
- Some good conductivity values were obtained.
- An overall material strategy has existed from the beginning to achieve most of the membrane targets.
- Some progress has been made towards achieving room temperature conductivity targets.
- Some experiments show that there is reason to believe mechanical strength will be adequate, and that additives will make a difference on performance.

Weaknesses
- Lack of partners.
- Macroscopic heterogeneity of membranes may lead to non-uniform current distributions in the cell.
- Alternative electrolytes may be difficult to perfect. Many barriers exist.
- More information on the materials or more thorough material evaluations needs to be provided to assess this work properly.
- There is no clarity regarding how certain targets will be met (e.g., freeze, additive stability).
- Samples described in the presentation must be more clearly marked. A sample code would help greatly.
- Mechanical testing limited to tensile strength and elongation measurements; mechanical testing needed for thinner membranes.

Specific recommendations and additions or deletions to the work scope

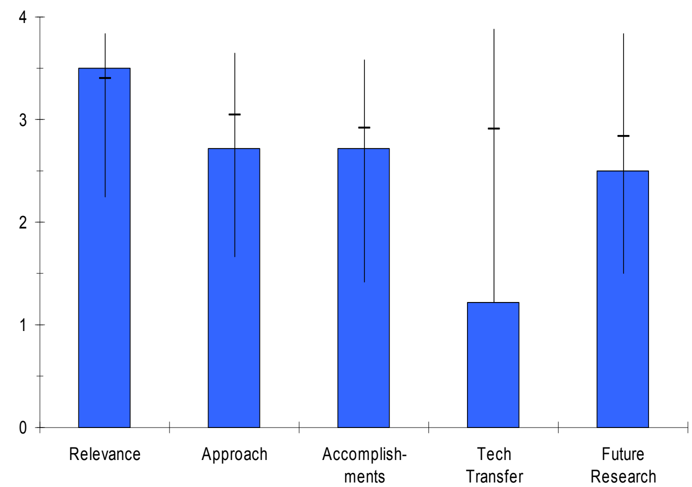
- Suggest inclusion of at least a broad description of the materials or materials properties to allow evaluation of project by reviewers.
- Project is early in its schedule. No recommendations at this time.
- Testing that assures stability of the additives in the membrane should be done in the next year.
- Obtain *in situ* mechanical cycling protocol from FreedomCAR Fuel Cell Tech Team.

Project # FC-19: Design and Development of High-Performance Polymer Fuel Cell Membranes
Ryo Tamaki; GE Global Research

Brief Summary of Project

The overall objective of this project is to design and develop novel polymer electrolyte membrane materials for fuel cell operation at high temperature (up to 120°C) and low relative humidity (RH) (25-50% RH). The objectives for fiscal year 2007 are to 1) design and synthesize a cross-linked system; 2) prepare a high acid density proton exchange membrane (PEM) in porous supports; 3) integrate hygroscopic inorganic additives; 4) evaluate membrane performance at different relative humidity; and 5) improve chemical and thermal stability.

Overall Project Score: 2.7 (7 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

- The development of high temperature/low RH membrane materials is highly needed for the successful commercialization of PEMFCs.
- The project addresses issues with fuel cell membranes and emphasizes hot and dry operating conditions.
- Project is aligned with DOE objectives and addresses DOE goals for PEM membranes.
- The project addresses most of the needs of DOE.
- Extended testing conditions are relevant to usage profile.
- Cost analysis is necessary for material modifications and additives addressed in the project and ensure those will be implemented with reasonable cost.

Question 2: Approach to performing the research and development

This project was rated **2.7** on its approach.

- The approach of random/block/grafted/cross-linked/reinforced HC materials is in-line with the industry's attempt to improve performance and durability of membrane materials based on these various membrane technologies.
- IP issues limit the ability for the reviewer to grasp the content at a high level.
- Barriers are addressed but approach is scattered. The PIs appear to have five or six different approaches – random copolymers, block copolymers, graft polymers, cross-linked systems, systems with porous supports, systems with additives, and want to try everything – not very focused.
- The approach is puzzling. The presenter says that there is an organic additive but the presentation describes an inorganic additive. The need for the porous support is also not explained. With the architecture of the polymers, there should be no need for this. It is puzzling.
- Unique and good approach of material modification to be sticking with target achievement.
- Weak at porous material downselection. Quantitative evaluation is necessary.
- Interactions among material modifications and additives should be tested.
- With the degree of swelling demonstrated, how can the support remain intact? Approach needs clarification.
- The approach taken in this project appears simplistic and has not benefited from advances made in other DOE sponsored research.
- Metrics for technical evaluation should be reviewed and aligned with DOE component technical targets.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.7** based on accomplishments.

- Progression of various generations show steady improvement in the material development in regards to proton-conductivity.
- No material durability has been investigated at this point.
- Have achieved acceptable conductivity compared to Nafion but no high temperature data yet.
- Claim year 2 milestone.
- Attempts with copolymer architectures have been unsuccessful.
- Cross-linking attempts have shown conductivity higher than or comparable to Nafion at high RH, but no real improvement at low RH – have not demonstrated conductivity at high temperatures.
- Significant progress appears to have been made. The presentation is a little unspecific and hence the lessons are hard to share.
- Promising performance data has been developed.
- Technical approach is not well thought out. More detailed characterization needs to be integrated into this program to determine viability of membrane.
- The project in early stages has demonstrated limited technical progress to date.
- Slide 17 – do not understand the advantage of reduced 'z' thickness change with significant x-y dimensional changes with cross-linking of the 4B polymer. This is the inverse of the technical objectives of other researchers so this appears to be disadvantageous.
- Recommend a technical go/no-go decision gate be added in the next phase/year to evaluate technical progress against DOE performance metrics.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **1.2** for technology transfer and collaboration.

- No collaborators outside of GE.
- Will eventually need a MEA manufacturer. Will eventually need a stack developer.
- Should interact with an established MEA manufacturer, automotive company or a university or national lab with extensive experience.
- Very poor. There is no sharing or collaboration. The results are cloaked as well. This project is close to the line of misusing public funds.
- Fuel cell testing and collaborations should be planned.
- Cost should be analyzed to evaluate materials and processes, third party evaluation is recommended.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.5** for proposed future work.

- Future work is in-line with the material development.
- Due to IP issues, it is difficult for the reviewer to fully understand and review this program at the level which is needed for the DOE.
- Continue more of the same.
- Cross-linked chemistry must have higher conductivity if placed in a porous support to make up for lack of conductivity of support. Also have stress issues between support and cross-linked ionomer, since these still appeared to swell quite a bit.
- Materials stability should be evaluated, e.g. retention of additives.
- Electrode interface characteristics should be investigated and recommend to pursue fuel cell testing.
- Needs to be expanded to and details provided about characterization to be performed.
- The proposed research is very general in nature and not directed at solving specific problems/issues.
- The project would benefit from staged metrics by which progress could be measured and activities directed at solving specific problems.

Strengths and weaknesses

Strengths
- Systematic approach to material development with the conventional technologies in membrane development.
- Brings a lot of different elements together which if performed correctly could result in a superior composite membrane.
- Systematic materials modifications.
- Material handling and testing capability.
- Understanding of fuel cell membrane requirement.
- Cross-linking polymers is a solid approach to adding sulfonic acid groups to polymeric chains to increase conductivity and strength.

Weaknesses
- Unclear how GE polymer will improve and with what technology as very little information was shared.
- There is too little disclosed to make a judgment on the approach, but many people have used inorganic additives previously with little success.
- Lack of collaboration.
- Have not shown improved conductivity at low RH yet.
- Approach lacks focus.
- NO collaborations.
- Interface characteristics between membrane and electrode.
- Project lacking fundamental mechanical integrity tests, Fenton's tests, and stability tests. The correlation between swelling (water uptake) does not correlate with the degree of cross-linking or sulfonic acid concentration and needs to be addressed. Measurement of swelling is primitive. Results to date are no any better than Nafion. Si should never be added to any PEMFC membrane (hydration layer is small and it is highly soluble in acid environment).
- This project update reflects a generic 'kitchen sink' approach, in which multiple approaches are being combined.
- Metrics by which technical progress can be evaluated could be improved.

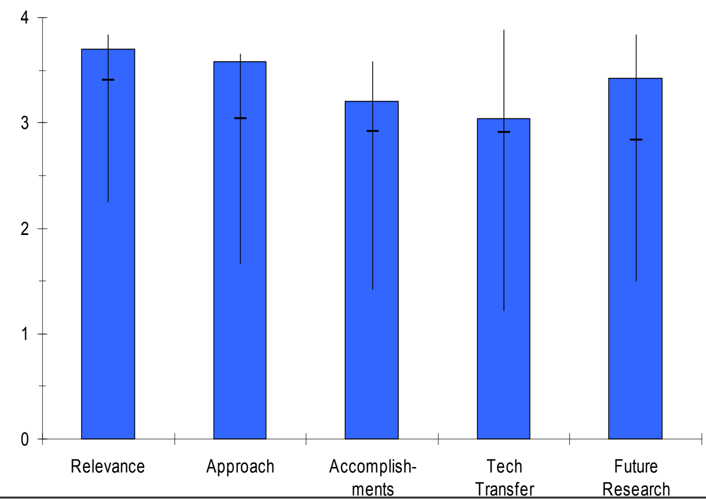
Specific recommendations and additions or deletions to the work scope

- Disclose IP after getting the IP protection – very difficult to gauge this project in the manner which is necessary.
- Eventually line up with MEA and stack developers.
- Establish collaborations with established expertise in the field.
- Develop proper collaborator to identify membrane/electrode interface characteristics and fuel cell testing.
- Pursue cost analysis on each materials modification addressed and ensure those are with reasonable cost.
- Technical metrics for each stage of development should be added into the project plan.
- Add metrics to evaluate cost potential of developed membrane technology.

Project # FC-20: Fluoroalkylphosphonic-acid-based Proton Conductors
Stephen Creager; Clemson University

Brief Summary of Project

Overall Project Score: **3.4** (5 Reviews Received)



The overall objective of this project is to provide new electrolyte materials for use in next-generation hydrogen fuel cell power systems, especially for transportation applications. The specific project objectives are to 1) synthesize and characterize new proton-conducting electrolytes based on the fluoroalkylphosphonic acid functional group and 2) create and apply new computer models to study proton conduction in fluoroalkylphosphonic acid-based electrolytes. The objectives for FY 2007 are to 1) synthesize and/or purify at least of 10 g each of one or more small-molecule fluoroalkylphosphonic acid electrolytes; 2) fabricate and validate an apparatus for measuring ionic conductivity of electrolytes at temperatures between ambient and 120°C and relative humidities between 25 and 100%; 3) develop classical force fields for and perform molecular dynamics (MD) simulations of low molecular weight fluoroalkylphosphonic acid electrolytes using the developed force fields; and 4) develop first generation of the multi-state empirical valence bond model (MS-EVB) for proton transport in fluorophosphonic acid.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.7** for its relevance to DOE objectives.

- The development of high temperature/low RH membrane materials is highly needed for the successful commercialization of PEMFCs.
- Project appears to focus on development of new, somewhat innovative electrolytes but stops short of actually synthesizing membranes for testing and evaluation.
- Project addresses the important task of identifying and qualifying a polymer candidate having acceptable conductivity over a broad range of RH levels and temperatures.
- The prospect of creating a phosphonic acid analogue of Nafion is particularly exciting. The utility of phosphonic acid groups at higher temperatures is almost as well-known as the leaching of phosphoric acid from membranes where phosphoric acid is bound only by hydrogen bonds.
- Mathematical modeling of the proton transport in the membrane is relevant to the progress towards developing membranes that conduct protons at lower humidity.
- The project is very relevant to the DOE program objectives in high-temperature, low humidity membranes.

Question 2: Approach to performing the research and development

This project was rated **3.6** on its approach.

- Fluoroalkyl-phosphonic acid based materials could provide a useful material to learn about proton-conduction mechanisms in a fuel cell.
- Synthetic approach is excellent.
- Modeling work has the potential to save time and money in membrane fabrication.
- Approach is directed toward the DOE targets of high-temperature, low-humidity PEMFC operation, but only emphasizes novel electrolytes rather than membranes – the ultimate measure of success would be incorporating

the new electrolytes into a membrane configuration. The project seems to stop short of the ultimate DOE objective of high-temperature, low-humidity membranes.

- The project includes a strong modeling effort.
- Good "scouting approach", with reality checks along the way.
- Screening test method for evaluating conductivities of liquid electrolyte candidates – good approach.
- Will the "work details" supporting the defined tasks be sufficient to resolve any deficiencies due to "benefit" assumptions for fluoroalkyl-phosphonic acids (weaker adsorption, higher oxygen solubility, chemically/thermally stable)?
- The sequential approach to transition from small molecules to monomers to the polymers themselves is reasonable.
- The one failing of the approach is that it neglects to include mathematical modeling of Nafion. How would the proton transport change from a perfluorosulfonic acid to a fluoroalkylphosphonic acid?
- The approach is very good. The concept represents a potential solution to high-temperature, low-humidity membrane.
- Understanding small molecule synthesis and simulating proton transport for low RH conditions is critical for success.
- The approach is a novel attempt to maintain adequate proton conductivity at low humidity conditions.
- Molecular modeling is being used to guide the synthesis of the fluoroalkylphosphonic acid electrolytes. Theory-guided synthesis provides a rational basis for certain pathways.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.2** based on accomplishments.

- Synthetic approach and modeling approach have thus far has shown success.
- Project is only 20% complete.
- To date, and given the limitations of project objectives, project appears to be off to a reasonable start with modeling refinement underway and several candidate electrolytes synthesized and initially tested.
- Good progress to date on several fronts (modeling, polymer synthesis, etc).
- Validation of conductivity apparatus for phosphonic acid has been completed.
- A different monomer has been synthesized than expected due to surfactant issues. Is there a way to use a different solvent in order to create the intended monomer? Is it possible to use the unintended monomer to enhance cross-linking for a new and unintended polymer (which would still be very interesting)? These issues should be explored.
- Equivalent weight is high.
- Good progress has been made on thermal stability.
- Progress has been made on reducing computation time for modeling.
- Good progress shown in difficult synthesis of small-molecule model compounds and trifluorovinyl ether monomers.
- Conductivity measurements are underway for several fluoroalkyl-phosphonic acids. The first results approach the 0.07 S/cm target.
- Molecular dynamics simulations are underway for two electrolytes. The simulations will be validated against NMR and conductivity measurements.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- Excellent team and collaboration of university professors.
- Will need industry support at some point to confirm the commercialization of this project.
- Several potential collaborators identified, but to date little actual collaboration accomplished. Perhaps this will come later.
- Project appears to have good selection of participant skills to achieve project goals, in particular computer modeling.

- Project is missing an industrial partner, who may be needed for resolving current and future polymerization issues.
- Collaboration with Kreuer bodes very well for this project.
- Industrial monomer synthesis experience could assist in removing hurdles concerning the monomer synthesis.
- Close collaboration between Clemson (synthesis) and University of Utah (theory) is evident.
- Two other collaborators on NMR studies are mentioned.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.4** for proposed future work.

- Future work is in-line with this membrane material.
- The target is difficult and needs to be followed very closely to see if this material can achieve the DOE targets.
- Future plans appear to be appropriate and well-throughout.
- Project tasks are clearly focused on targets and milestones.
- During the next phase of this project, the PI should identify qualified resources who might assist in resolving potential setbacks in preparing useful polymer samples – should that become necessary.
- The future work follows closely with the established approach, which is the strength of this project.
- Items that would improve the future work have already been mentioned (enhanced industrial collaboration, modeling of Nafion to compare against the fluoroalkylphosphonic acid).
- Future activity involves continuing synthesis and characterization of small-molecule model compounds and optimizing ionomer preparations.
- Molecular dynamics simulations will prevent the synthesis of compounds that do not exhibit adequate proton conductivity at low humidity. The work is highly relevant to the objectives of the DOE program.

Strengths and weaknesses

Strengths
- Good researchers with clear scientific approach.
- PI has a strong background in the required technical areas and is well prepared to address the project goals and objectives.
- Computer modeling efforts and analysis regarding expected properties and performance.
- Disciplined, meticulous approach.
- The most compelling chemistry amongst the DOE membrane projects.
- Depth of planning regarding the mathematical modeling approach.
- Progress made on synthesizing small molecules.
- Progress made on thermal stability.
- The project is an excellent example of the use of theory to guide synthesis of materials that show promise for good proton conductivity at low humidity and high temperature.

Weaknesses
- Assumptions are made which could end up being invalid – phosphonic acid vs. sulfonic acid strength and ability to operate at low RH and high temperature.
- Lack of industry support to validate the commercialization of this project.
- Project seems to stop short of actual membrane fabrication and testing.
- Current monomer end group "fixes" may not be suitable for successful aqueous emulsion co-polymerization.
- Too many assumptions, e.g., "fluoroalkyl-phosphonic acids should be chemically and thermally stable", etc.
- Hurdles have arisen in monomer and polymer synthesis.
- The synthesis of the various phosphonic acid-based electrolytes is likely to be difficult.
- Conductivity drops off significantly at low temperatures.
- While a rationale for the choice of a phosphonic acid membrane was presented, it was not supported by theory/calculations that showed that the phosphonic acid-based membranes are indeed better than sulfonic acid-based membranes.

Specific recommendations and additions or deletions to the work scope

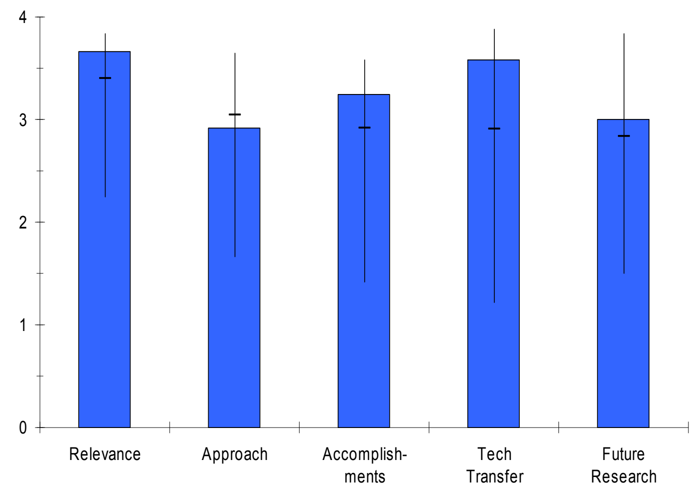
- Involve industry at some point to keep the project realistic in regards to scale-up and commercialization.
- Prepare membranes using the "best" electrolytes for test and evaluation.
- Select alternative monomer with end-group compatible with aqueous polymerization (e.g., one that does not need separate surfactant).
- Industrial collaboration on monomer synthesis.
- Mathematical modeling of Nafion as a baseline versus the fluoroalkylphosphonic acid polymer.
- The project should be continued long enough to allow for an adequate amount of research to determine the true potential of this approach even if the initial results do not meet the interim milestone of 0.07 S/cm at 25°C and 80% RH.
- Some thought should be given to the cost of producing these membranes.

Project # FC-21: Dimensionally Stable High Temperature Membranes
Cortney Mittelsteadt; Giner

Brief Summary of Project

The fiscal year 2007 objective of this project is to demonstrate, by the 3rd Quarter, membrane conductivity of 0.07 S/cm at 80% relative humidity at room temperature using non-Nafion materials. Samples will be prepared and delivered to the Topic 2 awardee. Samples will be prepared and delivered to the Topic 2 awardee.

Overall Project Score: 3.3 (6 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.7** for its relevance to DOE objectives.

- The goal of this project, to develop a proton-conducting membrane that can operate under low relative humidity conditions and high temperatures, is critical to the Hydrogen Fuel Initiative as it will decrease the cost and complexity of polymer electrolyte fuel cell power systems.
- Development of membrane for operation under hot and dry conditions.
- The project is relevant to DOE goals. If it turns out that water is necessary to achieve the goals then a higher EW is necessary. The swelling issue will then be critical. This approach is therefore good for dealing with this problem.
- The project addresses development of membranes for high temperature and low humidity. This is one of the key enabling technologies for automotive PEM.
- This project is very well aligned with the DOE H_2 Fuel Initiative.
- The Giner project aligns very well with the DOE objectives for high-temperature, low-humidity membranes.

Question 2: Approach to performing the research and development

This project was rated **2.9** on its approach.

- A reasonable rationale for the low equivalent weight, PFSA approach was given.
- The stability of membranes utilizing extremely water soluble, low equivalent weight ionomers is questionable.
- Using very low EW material in a stable 2D or 3D support.
- The premise is ok but it assumes water is always necessary. The humidifier problem will be horrendous. The use of the particular supports described is not immediately compelling. Will there be an adhesion problem?
- It is not clear why PFSA would provide the desired properties at high temperature and low humidity simply because it is held in a dimensionally stable matrix.
- It is not clear how separation of the monomer from the walls of the matrix would be prevented during cycling, especially humidity swelling and shrinking cycles.
- Approach is both appropriate and logical.
- The project focuses on understanding how support matrices can be used as a design option and technical feasibility of this option is well assessed.
- Excellent use of metrics to monitor and track technical progress.
- The approach is very good, innovative, and relatively low-risk. It is one of several different approaches taken by DOE to achieve membranes for high-temperature, low-humidity operation.
- It is focused on the technical targets required for automotive applications.

- The polymer support provides needed strength and stability for the incorporation of a low equivalent weight ionomer to increase conductivity at low RH.
- There is a need for adequate conductivity at very low ambient temperatures so that a fuel cell vehicle can achieve an unassisted start. Conductivity at low temperatures should be measured.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.3** based on accomplishments.

- The progress toward achieving the objectives of this project has been excellent and the Year 1 milestones have been achieved.
- Have investigated polyimide and polysulfone 30 µ hole/50% void space supports.
- Have demonstrated 700 EW PFSA in a fuel cell, but best at 100% RH.
- Polymerized Nafion monomer with co-monomers and impressively made the Nafion homopolymer.
- Good progress made.
- The project is fairly new so major progress is not expected.
- A significant portion of the progress seems to concern the matrix mechanical properties.
- The system shows no advantage over Nafion at low (25%) humidity (Slide 16).
- This project has elucidated the challenge and has made good progress in understanding methods of achieving the technical goals.
- Giner has demonstrated that their supported, dimensionally stable membrane achieved a conductivity of 0.1 S/cm at 30°C and 80% RH. This accomplishment meets the interim DOE target.
- Performance of the low equivalent weight-supported membrane in a fuel cell operating at 95°C and 25% RH was much worse than had been predicted.
- The supported membrane did not swell on the x-y plane and the ionomer did not separate from the support when dried.
- Giner appears to be making steady progress towards the objective.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.6** for technology transfer and collaboration.

- Excellent partnerships with GM and SUNY-ESF. Partnership with GM will facilitate the rapid incorporation of new membranes into fuel cell systems.
- Collaborations are a bit weak since GM owns the company.
- This project incorporates good coordination and guidance from GM.
- Close collaborations are evident with SUNY (new ionomers) and with GM (automotive targets for membranes).

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- Continue to synthesize new ionomers.
- Expand work to 3D supports.
- Future work logically follows progress to date.
- More emphasis should be put on monomers than on the matrix.
- The planned work is appropriate. An evaluation of solubility of impregnated polymers in the DSM might be included if it is viewed as a risk item by the project team.
- Future plans are focused on developing even lower equivalent weight ionomers to achieve 0.1 S/cm at the low humidity condition.

Strengths and weaknesses

Strengths
- Support architectures.
- Access to novel PFSA polymers.
- Well-focused and directed effort.
- The effort is well focused and driven by a clear understanding of automotive requirements.

Weaknesses
- It is not clear how this really differs from work at Gore and other MEA manufacturers using reinforced/supported membranes.
- Need more polymer characterization in the program. Adhesion will be a problem.
- A clear path to synthesizing an ionomer with low enough equivalent weight to meet the conductivity requirement yet remaining stable is not evident.

Specific recommendations and additions or deletions to the work scope

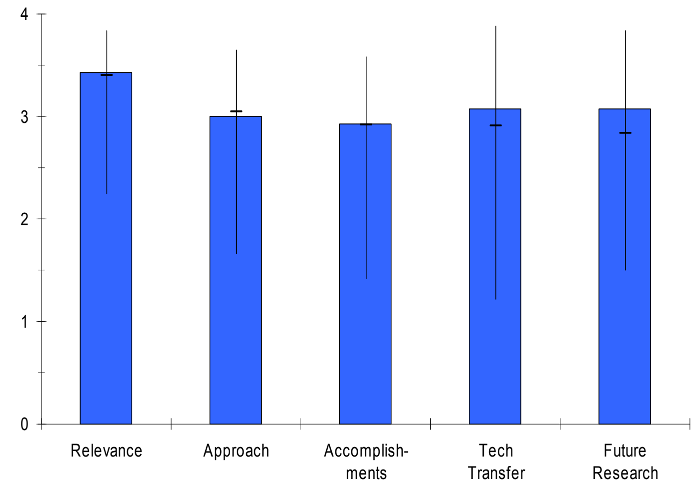
- Fuel cell work should be postponed until after the Go/No-Go decision has been passed.
- The laser-drilled 2D support is impractical and should be used to direct research using the 3D support.
- Giner needs to balance the need to understand the poor fuel cell performance against the need to develop new ionomers with low equivalent weight. Significant resources should not be diverted from ionomer development to understand the fuel cell performance issue at this time.

Project # FC-22: New Proton Conductive Composite Materials with Co-continuous Phases Using Functionalized and Crosslinkable TFE/VDF Fluoropolymers
Serguei Lvov; Penn State

Brief Summary of Project

The overall objectives of this project are to 1) contribute to DOE efforts in developing a high temperature proton exchange membrane (PEM) for transportation applications and 2) develop a new composite membrane material with hydrophilic inorganic particles and TFE/VDF polymer matrix to be used in PEM fuel cells at -20 - 120°C and 25-50% relative humidity (RH). The Year 1 objectives are to: 1) synthesize inorganic proton-conductive materials; 2) develop chemistry for functionalized TFE/VDF polymers; and 3) develop membrane fabrication methods.

Overall Project Score: 3.1 (7 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.4** for its relevance to DOE objectives.

- Addresses the DOE goal of developing a high temperature, low relative humidity membrane for PEM fuel cells.
- The project is highly relevant to the DOE's objectives and to support the President's Hydrogen Fuel Initative.
- Project aligns to multiple challenges of the hydrogen vision.
- New material development is important.
- This project addresses the need for high temperature membranes.
- Relevant.
- The development of composite membranes with hydrophilic inorganic particles in a functionalized fluoropolymer matrix is one of a number of diverse approaches being taken by DOE to meet the advanced membrane targets. The project is very relevant to the DOE objectives related to high-temperature, low RH membranes.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- The technical approach focuses on the development of a composite membrane - a unique and innovative approach.
- The project is for 5 years. The project addresses the polymer membrane electrolyte issue. The technical approach for the program is excellent. The tasks are clearly presented.
- The project is well organized and divided into manageable tasks.
- To provide a membrane that meets DOE targets, it is likely that more will be required than hydrophilic additives. It is not clear that the polymers being used here will provide the required conductivity or durability to do this. Nafion does not.
- Achieving percolation will be difficult if matrix is not conductive.
- Blending with Nafion—unlikely to help, especially if the same equivalent weight is used.
- The proposed technique will make it difficult to get small particle sizes.
- The approach has multiple pathways to achieve the desired conductivity including different avenues without Nafion. This increases the chances of success.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.9** based on accomplishments.

- Given that the project is only 20% complete, progress has been good.
- Several initial composite membrane samples have been synthesized.
- Testing/characterization instrumentation in place with initial conductivity measurements done.
- The project was started in May 2006. It is too early to make a judgement for technical accomplishments at this time. However, the project progress is excellent.
- Project has accomplished year 1 tasks, but more clear alignment to DOE technical targets should be shown.
- There is nothing to suggest that the polymers used have adequate chemical stability. The path to high conductivity under hot, dry conditions needs to be explained more fully. The current conductivity is quite low.
- None of the approaches appear to come close to Nafion.
- No mention of durability.
- The accomplishments by the PSU team have been pretty significant. Several inorganic additives have been synthesized, the most promising of which is zirconium phosphate.
- The team prepared several membranes with these additives in a fluoropolymer matrix and measured the conductivities of the composite membranes. Initial results showed conductivities at 120°C and 70% RH to be about 0.01 S/cm. This conductivity was achieved with poly VDF-CTFE/Nafion blends.
- Conductivities of the non-Nafion-containing polymer composites were about three orders of magnitude less than the those containing Nafion.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.1** for technology transfer and collaboration.

- Conductivity instrumentation provided by BekkTech—it wasn't clear whether this was a collaboration or just a procurement.
- ORNL was mentioned as a collaborator in characterization, but there was no indication of interactions with ORNL to date - perhaps this is to come later in the project.
- The project was started in May 2006. It is too early to transfer technology to industry at this time.
- Collaboration appears to be primarily within Penn State.
- Consider collaboration with membrane supplier.
- A good team has been assembled for this project.
- A good team in place.
- Collaboration with ORNL and with BekkTech is in evidence.
- Many stakeholders provided input in formulating the baseline assumptions and defining market requirements and criteria for acceptance.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.1** for proposed future work.

- Project appears to be off to a good start - future plans appear to appropriate and reasonable.
- Based on the presentation information, the future research work is clearly presented and technical approaches are reasonable.
- Future work continues overall solid plan.
- Important to reach go/no-go decisions.
- Eliminating Nafion has been proposed, but given the low conductivity of the alternates, unclear how realistic this is.
- Future plans call for continuing to modify materials and process conditions in an iterative fashion until the conductivity requirements are met. A rationale for specific modifications should be developed.

Strengths and weaknesses

Strengths

- A high risk approach, but with a potential high reqard.
- PI is knowledgeable, underatands the challenge, and has structured a meaningful research project and clear, well-defined objectives.
- The PI, co-PI, and coworker have excellent R&D experience for polymer membrane electrolyte chemistry.
- Well organized.
- Approach is novel.
- The PSU project team has succeded in casting composite membranes. With some Nafion in the blend, conductivities approached that of Nafion.
- New mechanisms for conduction through the interfaces in composite materials.
- The work was well received by the community.

Weaknesses

- Stability of the composite membrane may be an issue.
- SiOH attack may adversely affect stability and membrane lifetime.
- Water may hydrolyze the silane functional group.
- The polymers used may not have adequate chemical stability. The path to high conductivity under hot, dry conditions needs to be explained more fully.
- Focus appears to be on testing a number of additives, none of which seem to come close to milestones. An alternative approach (Plan 8) would be useful.
- Durability not addressed.
- Without Nafion the conductivities of the composite membranes were quite poor.

Specific recommendations and additions or deletions to the work scope

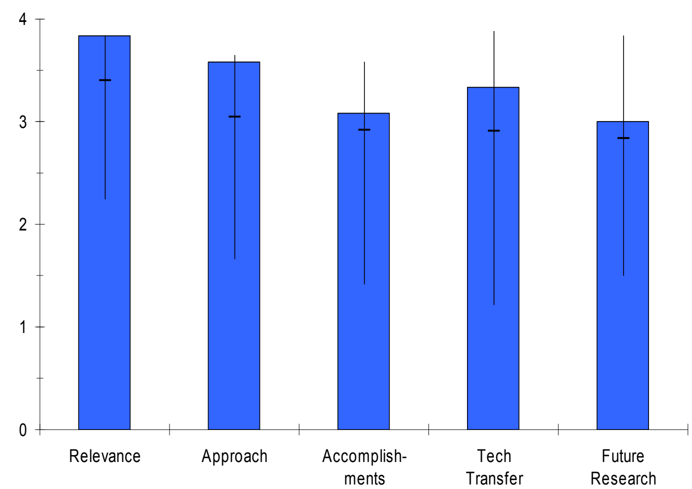
- This project just started the second year, project progress is excellent. No action is need at this time.
- Reduce the number of additive options.
- The project could benefit from theory/simulation of the conduction mechanism to see how it matches with experiment.

Project # FC-23: Advanced Materials for Proton Exchange Membranes
James McGrath; Virginia Tech

Brief Summary of Project

The overall objective of this project is to design, identify, and develop the knowledge base to enable proton exchange membrane films and related materials to be utilized in furl cell applications, particularly for H_2/air systems at 120°C/low relative humidity (RH). Thermally, hydrolytically, and oxidatively stable aromatic ionomers with high T_g, ductility, and controlled hydrophilicity are required. The PI will synthesize linear multiblock hydrophobic/hydrophilic copolymers.

Overall Project Score: 3.3 (6 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.8** for its relevance to DOE objectives.

- This works aims to improve the performance and durability of low cost membranes.
- New polymeric systems should be a component of the longer term approach to address the key objectives of the DOE program with respect to stack life.
- The program addresses an important aspect for development and introduction of automotive PEM fuel cells.
- Relevant.
- This project is directly relevant to key component technology goals of the President's Hydrogen Fuel Initiative.
- The project objective is critical for realizing a renewable energy economy.

Question 2: Approach to performing the research and development

This project was rated **3.6** on its approach.

- All approaches make sense (block copolymers, lower x-y swelling, Flory-Huggins modeling).
- PI is conducting all the right *ex situ* tests (conductivity vs. RH, dimensional stability, mechanical tests, structural analysis).
- Approach is sound – block co-polymers have a chance of evolving into a viable membrane with tailored properties.
- Synthesis route and supporting activities approach are appropriate for this level of funding and commitment.
- Understanding of mechanical properties and water transport and conductivity mechanisms is a key part of this effort.
- The approach builds on previous work at VA Tech.
- Very elegant – a good mix of fundamental and applied science.
- This project has a logical approach to understand and develop novel polymer materials.
- Good understanding of key material attributes has been demonstrated by the project team.
- The PI provided a noble approach for low relative humidify operation understanding property/structure relationship.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.1** based on accomplishments.

- Significant progress in conductivity and swelling reduction.
- Still need to demonstrate fuel cell performance and durability.

- Too early to really assess the results but the materials under study and the approach will provide greater insight with time.
- Conductivities of new materials are comparable to Nafion.
- Mechanical behavior of some of the new materials has been evaluated and compared to Nafion.
- Water retention of the new materials is higher than Nafion.
- Low RH results are very impressive – certainly a step in the right direction. Same with water retention.
- This project is focused on developing novel materials and leverages from previous DOE-sponsored R&D by the same team. It has demonstrated good to outstanding technical progress as well as deeper understanding of the polymer design factors.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.3** for technology transfer and collaboration.

- PI has taken advice of OEMs.
- PI could benefit from some external testing of the membranes.
- None.
- Team includes LANL, Giner, and Hydrosize.
- Good team.
- This project has good collaborations, however these were not well highlighted in this review presentation.
- Contributions from the partners were not discussed.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- PI should include fuel cell performance and durability testing in future work.
- Prof. McGrath is a solid contributor and what is proposed is exactly what needs to be done.
- Future research builds on progress and addresses issues relevant to attainment of project and DOE goals.
- Should include chemical degradation! Otherwise sound.
- The proposed work is focused on polymers but not on creating fuel cells with films made from these polymers.
- Proper plan has been laid out for the next step.

Strengths and weaknesses

Strengths
- PI shows excellent combinataion of synthesis, characterization, and modeling skills.
- Solid team and lots of history and experience with such polymeric materials.
- Innovative approach – examines most angles.
- Excellent PI and team.
- Strong level of innovation in this project.
- New approach to formulate fuel cell membranes.

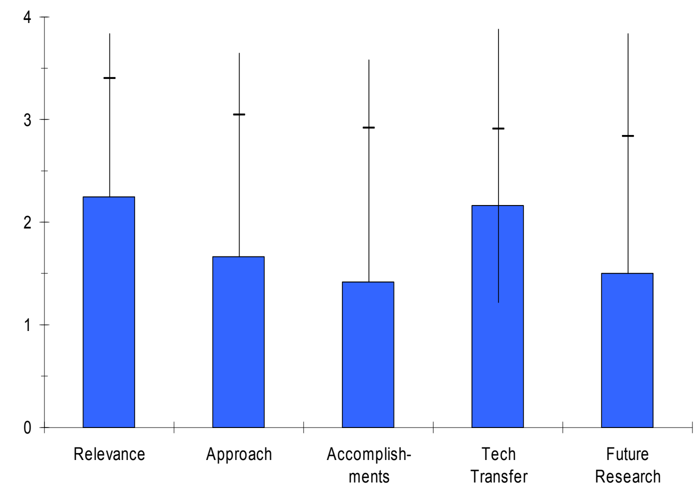
Weaknesses
- Materials unlikely to meet 2015 DOE performance targets.
- Use of tensile tests as sole measure for mechanical strength.
- Durability not yet addressed.

Specific recommendations and additions or deletions to the work scope

- PI should include fuel cell performance and durability testing in project scope.
- PI should consider doing cost of production study of most promising membranes.
- Durability tests should be introduced.
- Addition - an assessment of these novel polymers against key performance and failure modes (such as wet/dry hydration cycles) to be used as a metric to measure progress.

Project # FC-25: Center for Intelligent Fuel Cell Materials Design Phase 1
Denise Katona; Chemsultants International

Overall Project Score: 1.7 (6 Reviews Received)



Brief Summary of Project

The objective of this project is to develop novel polymer architectures capable of 1) improved mechanical stability vs. Nafion (117) 212; 2) improved conductivity vs. Nafion (117) 212; and 3) ≥ 120°C/ ≤ 50% relative humidity (RH) operational capability (4,000 hours). Additionally, the project aims to identify new solution casting methodologies for thin, roll-to-roll membrane formation. This could consist of thin single layer membranes, discrete multi-layer membranes and reduction in stack component cost (membrane).

Question 1: Relevance to overall DOE objectives

This project earned a score of **2.3** for its relevance to DOE objectives.

- The pursuit of improved membranes for high temperature and low RH conductivity is reasonable. However, the project is following routes thoroughly explored as much as 10 to 15 years ago by the research community. The work presented is essentially "reinventing the wheel" and not using the most current and evolved technology in the area. The exception to this is the novel additives that are being pursued, however this is a fairly minor addition to the state of art in this area.
- Addresses new membrane materials.
- Addreses manufacturing needs of the hydrogen economy.
- This project involves sulfonation of a commercial polymer. Little new knowledge is generated for the DOE objectives. It may demonstrate the company's capabilities but does not contribute to new knowledge.
- This project is relevant to the objectives of the HFCIT program as addressing the important issue of high temperature membrane.
- Insufficient targets for either automotive or stationary application.
- For automotive, performance and materials stability at lower temperatures are required.
- Unclear project objectives, long-term research project or short-term optimization based on available materials?
- The technical objectives related to development of new materials are highly relevant to DOE goals. The objectives to identify new solution casting film manufacturing processes are not relevant as these are well established and mature.

Question 2: Approach to performing the research and development

This project was rated **1.7** on its approach.

- Post-sulfonation of poly ether sulfones has been done in the past. The community generally favors polymerization of sulfonated monomers at this time as the resulting materials tend to have lower water uptake and higher conductivity. Combining additives to polymer electrolytes is a viable approach to improving high temperature membranes, however little understanding of the system or of prior work in this area has been demonstrated in the presentation.
- Polymer modification.
- Addition of nanoparticles.
- Optimization of loadings/layers.
- Manufacturing.

- This project appears to be a demonstration of capability. It provides little new insight. What is the purpose of the nanoparticles?
- The approach used in this project is not innovative; this applies to both "modification" of polymers and the use of "additives".
- The advantages of the approach taken remain unclear.
- Benefits from the use of SEM, TEM and other microscopic techniques are not obvious at the moment.
- Further investigation is necessary to identify proper metrics for performance target. Water uptake is not sufficient to characterize to achieve proton conductivity target.
- Not meaningful to investigate the manufacturing process prior to characterization of materials.
- For fuel cell testings, materials and MEA design (other than membrane materials) should be defined and identify correlation between membrane material and fuel cell performance should be identified.
- Unclear criteria to use additives A and B.
- This project has insufficient focus on the key performance metrics and premature focus upon manufacturing methods. The polymer platform chosen does not appear to be adequate in terms of its basic properties and the separation of the effects of the nanoparticle additives from those of the base polymer platform was not highlighted (beyond the *ex situ* properties table which is insufficient).

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **1.4** based on accomplishments.

- Conductivity and fuel cell performance reported are regressing from current state-of-the-art already demonstrated for similar materials. Roll-to-roll processing may be of some value, however the materials being investigated are of too inferior a quality to make much difference at this time.
- Very little data was presented on conductivity, and none was presented as a function of relative humidity.
- There appears to be little evidence that any significant improvemnets in conductivity have been achieved at hot or dry conditions.
- Fuel cell testing using bad MEAs and no evidence of reproducibility or error analysis.
- Manufacturing of polymers with minor improvements will not be useful.
- The project has made polymer films. Unfortunately, they do not work. The results show little chance of reaching the goals. The presenter displayed ignorance of how a fuel cell works by not knowing if the polymer was used in the electrode.
- Subpar performance data obtained with the reference Nafion membrane make all performance comparisons difficult.
- Difficulties with performance comparisons notwithstanding, polarization plots indicate significant performance drop relative to Nafion, especially at low current densities.
- Tensile strength drop at high sulfonation levels is somewhat disappointing, especially in the context of the stated intent to obtain polymers with improved mechanical stability vs. Nafion.
- Fuel cell performances are insufficient (low performance to proceed).
- Effects of additives should be evaluated.
- Even though the project is 65% complete, there is little demonstrated progress against the key technical performance goal!
- This project is looking to develop a suitable polymer system for higher temperature, lower RH operation but there is only relatively poor *in situ* performance demonstrated at relatively “gentle” operating conditions (80°C and 50% RH).

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.2** for technology transfer and collaboration.

- Michigan Molecular Institute and Case Western Reserve University are collaborators. Coordination seems reasonable, however the experience of this team appears insufficient and the addition of more experienced researchers in this area could greatly improve the project.
- Collaboration with Michigan Molecular Institute, GrafTech, and Case Western.

- On paper this looks good. However, if the investigator really had interactions with CASA, she would have been able to answer some critical questions.
- The flow of information between Chemsultants and Case Western pertaining to the materials testing should be improved, including such important issues as electrode compositions, possible reasons for poor fuel cell perfomance, etc.
- Disconnection between materials test and fuel cell testings.
- It appears that better overall leadership and prioritization of activities between partners would help this project focus on the key risk areas.

Question 5: Approach to and relevance of proposed future research

This project was rated **1.5** for proposed future work.

- Future work is more of the same, focusing on approaches demonstrated by others that have not led to materials that were sufficient to meet DOE technical targets.
- New polymers.
- New additives.
- Fuel cell testing – premature.
- Manufacturing – premature.
- Do not know where this is going.
- Poor performance to date makes the need for scale-up questionable at this time.
- Future work should focus on major improvements to membrane/MEA performance.
- Materials characterization to achieve the target is insufficient to larger scale testings and manufacturing process study.
- Given the future work stated, this project has low probability of reaching its technical goals with the remaining budget and time. Focus on achieving technical performance goals (higher temperature, low RH conductivity) should be prioritized in favor of efforts on low technology risk activities such as film manufacturing.

Strengths and weaknesses

Strengths
- Few.
- Nice use of novel nano-inorganic functionalized additives.
- Manufacturing.
- Demostrated manufacturing by two different techniques.
- Materials optimization for hydrocarbon-based polymer electrolysis.
- Consideration of synthesis and film fabrication provides valuable direction to the core material development.

Weaknesses
- Too much emphasis on fuel cell testing and manufacturing of materials with few advantages over exsisting materials.
- Investigator does not appear to know how a fuel cell works.
- Very little achieved in spite of very significant funding.
- Response to questions was not the strongest part of the presentation, among others, indicating certain disconnect between Chemsultants International and partners at Case Western.
- Understanding of fuel cell membrane requirements and metrics.
- Insufficient focus on core material properties.

Specific recommendations and additions or deletions to the work scope

- This project provides almost no value to the community and the funding for the project would be much better spent elsewhere.
- Emphasize investigations of composite membranes and conductivity testing.

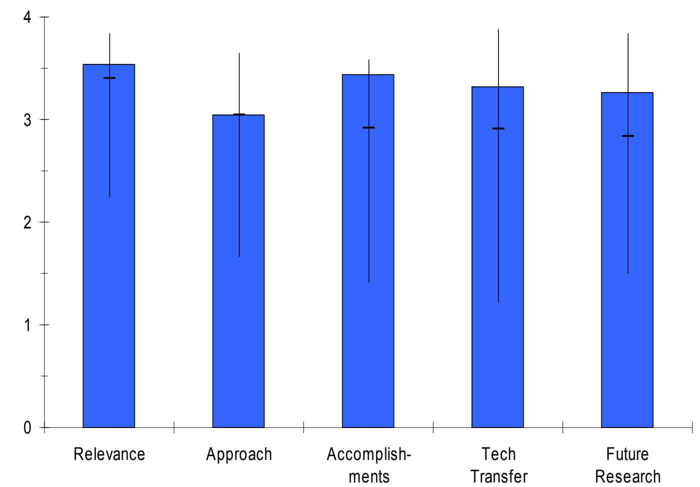
- Do not perform fuel cell testing or manufacturing on these materials. The project is too short and the emphasis should be on materials discovery.
- This project should be terminated.
- Much better performance shoud be demonstrated before any effort is invested in scale-up and manufacturing; without a major improvement in MEA performance, this project should be terminated.
- An addition of a sound cost analysis would help better understand benefits of the approach.
- Basic evaluation of membrane stability is needed.
- Focus on membrane materials characterization for the rest of the project time.
- Further investigation to identify proper metrics for material characterization, other than water uptake, e.g., dimensional stability, etc.
- Incorporatation of feedback from fuel cell performance testings.
- Add metrics and project technical gates for core material performance metrics, consistent with DOE technical goals.
- Reduce or delay activities focused on low technical risk activities such as film manufacturing.

Project # FC-26: Economic Analysis of Polymer Electrolyte Membrane Fuel Cell Systems
Kathya Mahadevan; Battelle

Brief Summary of Project

The objective of this project is to assist DOE in developing fuel cell systems by analyzing the technical, economic, and market drivers of direct hydrogen proton exchange membrane fuel cell (H-PEMFC) adoption. Support in 2006 included 1) market segmentation of 1-250 kW H-PEMFC into near-term (2008) and mid-term (2012) market opportunities; 2) lifecycle cost analysis of H-PEMFC and competing alternatives in near-term markets; and 3) market opportunity assessment of H-PEMFC in near-term markets.

Overall Project Score: 3.3 (4 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

- The project objectives are very closely related to DOE objectives.
- The market analysis data that will be collected in this project are very critical to understand the market.
- The cost comparison data resulting from this project will be very crucial for fuel cell manufacturers for developing their technology.
- The market opportunity data from this project will give the clear understanding on the market readiness for fuel cell technology.
- The cost modeling will be valuable to determine the possibility of success in different market segments, such as forklift, portable, federal markets, etc.
- DOE is coming to an increased realization that early adopters in "premium power" markets will provide private-sector market pull (demand) for advancement in fuel cell technology (i.e., through private sector investment). These technical advancements could then "spill over" into the more demanding automotive application.
- This project is a thorough and comprehensive study to determine market niches for which fuel cell technology could be competitive today, thus providing seeds for technology development within the private sector.
- Near-term market understanding is a critical stepping stone to the transportation sector and a clear independent analysis is in full support of the DOE objectives.
- All fuel cell manufacturers are likely doing similar studies without government help.
- Much PEM system technology is not the same for automotive and non-automotive applications.
- Not much can be gained from this study to help project goals.

Question 2: Approach to performing the research and development

This project was rated **3.1** on its approach.

- Company sampling and information collection process was adequate.
- The approach to the market and cost data collection and analysis techniques was adequate.
- The approach to the development of market penetration modeling was good.
- Near- and long-term market selection process through information collection was adequate.
- The data on the reliability expection of the customer companies can be included as a part of this model.
- The "Approach" slide (#4) is eye-candy for management. In reality, the "approach" of this project must be judged on the strength of its research.

- The PI demonstrated a thorough and comprehensive research program that provides a solid foundation for conclusions ultimately reached.
- The topic is really broad so it is reasonable and understandable that the scope had to be limited in the quantitative analysis to only PEM fuel cells and to the fuel cell specific markets.
- Suggest that consideration be given to speaking to financial stakeholders such as venture capitalists in this sector or to investment banks that cover some of the public fuel cell companies to see how they view the market.
- In the report, some qualitative analysis may be appropriate on the applicability of other fuel cell technologies like solid oxide or DMFC.
- Even much larger numbers of survey responses than involved in this study are known to be unreliable. Survey answers also are known to depend on the questions and how they are phrased.
- There did not seem to be any innovation or significant original thought in the approach.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.3** based on accomplishments.

- Seventeen completed surveys and three meetings for USFCC.
- The outcome of the H2A model for comparison between fuel cell and alternate power seems to be realistic.
- Capital cost barrier for H-PEMFC implemetation was addressed.
- Forklift market analysis (cost, life, battery comparison) will be very useful to fuel cell community.
- Reliability and capital cost for forklift implementation was determined.
- Market penetration analysis for forklift products will be very useful for fuel cell developers.
- The PI demonstrated detailed results for the forklift and material handling equipment, and indicated that similar analysies (for other markets) were part of the final report, available to DOE.
- A note on slide #19, "Reduce[d] vehicle repairs due to fewer moving parts." True – the repairs may not be due to moving parts, but what available data justifies a claim that one technology would require fewer repairs, regardless of cause?
- Very thorough analysis was done. One comment for improvement is to clearly articulate what of the results was different or improved upon from last year. It feels like I heard most of this before.
- Neither the limited modeling nor the few resulting projections represent significant accomplishments.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.1** for technology transfer and collaboration.

- The data and model out of this project will be available to public.
- Considerable collaboration between the fuel cell developers and customers from different market segments are being developed through this project.
- The data will be shared with future fuel cell developers to give them the realistic view on the market.
- The nature of this work was to have extensive interaction with potential customers and suppliers during the research phase.
- The accumulated data and conclusions of this project would be best reviewed by opening them to validation by all stakeholders (i.e., as part of the formal process, both prospectively (before new market adoption) and retrospectively (after field experience in new markets is obtained).
- Strong outreach to industry and other technical stakeholders.
- There is little evidence of collaboration except perhaps with NREL.
- The individuals contacted and/or surveyed and/or participated in discussion groups hardly represent technology transfer or collaboration.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.4** for proposed future work.

- The same approach will be taken to collect VOC data and develop models for federal and portable markets.
- The study will be restricted to H-PEMFC for portable markets, unless DOE advices otherwise.
- DMFCs for portable markets won't be considered for future work.
- The forklift market penetration and viability analysis will be a good tool to develop future models.
- The PI is wise to address EPACT requirements in future work.
- Clearly articulates what will be done for the balance of 2007 and within the current scope of funding.
- Would have liked to see some specific recommendations for how they could take this research to the next level of detail in out years if more funding were to be made available.
- This is something that needs to continued to be funded either through Battelle or another contractor.
- No future work proposed beyond continuing current activities.

Strengths and weaknesses

Strengths
- Significant amount of VOC data had been collected.
- The data collection and analysis methods were very thorough and systematic.
- Through the forklift market study, a good tool has been developed for future implementation into different market segments.
- Comprehensive research.
- Thorough analysis.
- Inclusion of sensitivity analysis (slide #16).
- Structured analysis that clearly states the assumptions and characteristics of the work performed.

Weaknesses
- Only six months (March 2007 to September 2007) is left for the completion of 36% of the project.
- Lack of stackholder feedback, both immediate and based on operational experience.
- Could add additional stakeholders like investment community to the data collection to solicit other points of view.
- Work is likely a duplication of efforts ongoing or already completed in the fuel cell industry.
- Low power systems with completely different duty cycles would not likely provide significant aid to vehicle fuel cell system development.

Specific recommendations and additions or deletions to the work scope

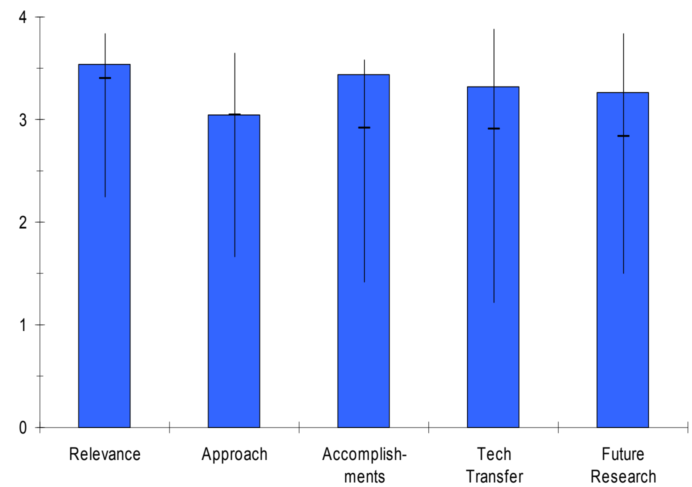
- Important data, such as customer views on reliability and maintainence expectations of fuel cells can be incorporated in the study.
- Although DMFCs are not a part of hydrogen economy, they are PEMFC technology. Therefore, DOE should consider using DMFC applications for portable market as a subject for this study.
- There is an inconsistancy between slide #3, in which they say that DOD applications are out of scope, and slide #7, which says that the scope includes DOD markets.
- I would recommend a more detailed but much broader project in the future that focuses on 2-3 very specfic market segments like fork lift trucks and perhaps telecom backup power. In these scenarios, competing technologies and other market barriers to entry could be further enhanced in a more narrow scope of work.
- Do not continue this type of project beyond the current contract.

Project # FC-27: Direct Hydrogen PEMFC Manufacturing Cost Estimation for Automotive Applications
Stephen Lasher; TIAX

Brief Summary of Project

The overall objective of this project is to perform a manufacturing cost assessment of an 80 kW direct H_2 proton exchange membrane fuel cell (PEMFC) system for automotive applications. The objectives for fiscal year 2007 are to perform 1) a high-volume cost projection for a PEMFC system using current performance/ cost assumptions; 2) a bottom-up manufacturing cost analysis for balance-of-plant (BOP) components; and 3) evaluation of economies-of-scale impacts on the stack and BOP and of technology/cost breakthroughs needed for systems to meet 2010 and 2015 targets.

Overall Project Score: 3.3 (6 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

- Fuel cell cost is the number one barrier. Understanding cost drivers is critically important to achieving the DOE objectives.
- Addresses one of the top three barriers, cost.
- That's very important for the automotive OEMs as well as for the suppliers to see, if they really can make the fuel cell car an economic reality.
- Addressed stack as well as system cost targets from the DOE based on 500,000 units a year.
- Very important to track progress towards the fuel cell cost goals using an independent body to do so.
- We need to know where we are relative to fuel cell cost goals!
- In general, the effort of estimating fuel cell system costs is highly relevant.
- The concept of using 3M NSTF technology at high volume in 2007 is not at all realistic. However, there is benefit in using this technology for a cost estimate since it is the only technology that moves away from the "business as usual" of using high surface area carbon supports.
- Some system assumptions are unrealistic, although the difficulty in obtaining proprietary system information is recognized.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- Very rigorous approach, based on well-established corporate expertise for conducting cost analyses, coupled with a good understanding of the technology. Approach includes bottoms-up costing and developer feedback.
- The TIAX proprietary model for costing the stack components, if independently vetted, is critical for accuracy.
- Close collaboration with ANL modelers is excellent.
- Good to look also at hydrocarbon membranes.
- I have some reservations about basing this cost estimate on 3M's alloy catalyst exclusively. I think it should be captured as a footnote whenever the cost estimate is referenced. On the other hand, I don't have a better idea.
- System assumptions are scheduled to be updated this year, but should be challenged this year. It is doubtful that the 3M MEA technology requires external humidification devices on both gas lines.

- Given the specificity of the assumptions, a sensitivity analysis is in order and should be shown in the presentation.
- Balance-of-stack components are greatly neglected, although the difficulty in obtaining information is recognized.
- The merits of performing a cost analysis using 3M technology are real and are commendable.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.4** based on accomplishments.

- Excellent progress in updating the cost projections as the technology improves and material costs, especially platinum cost, change. Design basis is up-to-date, assumptions are clearly presented, and the results are completely defensible.
- This project builds on the previous year's progress. This year's analysis, based on new feedback from ANL systems modeling, has been accomplished relatively quickly.
- Key result is that by lowering the MEA costs, the overall sytem costs are reduced and now the balance of plant costs become an increasing portion of the cost.
- Progress from stack to BOP is in progress.
- Includes different grades of humidification.
- Good articulation of specific changes from previous work and what the drivers for those changes are.
- Slide 7: I think TIAX is talking about the price TO the OEM, not the price an OEM will charge.
- Current cost estimate relies heavily on the 3M alloy catalyst, the cost, performance, and durability of which remains to be proven. Not that I have a better suggestion; just a caveat on the cost estimate that should be kept in mind.
- Leaving aside any perceived issues with the approach, the technical delivery is excellent. It is understood that copious MEA processing details are proprietary to 3M and they are not expected to be shown here.
- DTI showed an active investigation into graphite versus metal plates. The same should have been done here.
- A number of assumptions are not well understood, such as the motivation for woven GDLs, the motivation for two stacks per system and other details.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.3** for technology transfer and collaboration.

- Excellent interaction with system developers and component manufacturers to ensure reasonable inputs. Good dissemination of results at review meetings and with the Fuel Cell Tech Team.
- Good to collaborate with Argonne.
- MEA supplier data taken into account, important.
- Excellent collaboration with industry to help pull the information together.
- TIAX has made a good effort to get industry input. Unfortunately, industry is reluctant to provide cost data, so this is a very difficult area in which to work.
- The project is entirely dependent upon collaboration, so the collaboration level is already high.
- Answers to questions revealed that there is too much dependence upon National Laboratories. Greater industry collaboration (if possible) should be expected.
- As system update is performed in 2007, collaboration should be expanded to investigate a variety of vendors for system components.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.3** for proposed future work.

- Plans for future work will focus on balance-of-plant costing. Plan for getting feedback from developers and stakeholders is good.

- Very good to continue to revaluate, from the bottom up, and get more stake-holder feedback, on all the assumptions.
- More feedback on the validity of the bottom-up models is recommended.
- Important to also factor in durability advantages/disadvantages of the system subcomponents, using real data from similar types of systems.
- Feedback will be incorporated, important.
- Should publish the results in the peer-reviewed literature.
- Updating the BOP cost assumptions is critical to this project and this need is clearly identified.
- The need for sensitivity analyses is also critical and the investigators acknowledge that.
- Some of the questions identified additional areas of study, such as MEA component recycling and supply chain analysis. The presenters stated that they had studied supply chains, but the criticalities within individual component supply chains were not shown.
- Some evaluation of stack assembly time and conditioning time should be included.

Strengths and weaknesses

Strengths
- Experience with this kind of analyses.
- Great database on material and manufacturing cost in BOP components.
- Sensitivity is included.
- Good job of taking a very varied group of design parameters and distilling them down to something that is easy to track from a baseline and update approach.
- Excellent, thoughtful analysis of cost drivers.
- Cost analysis on a specific technology with advanced catalyst supports.
- Stack assumptions have been modified to reflect advances in components.
- Collaborations with some system component manufacturers to understand costs.

Weaknesses
- No OEM included to deliver updates on system design.
- Relies on cost estimation from suppliers on key components; e.g., membrane or bipolar plates.
- I do not think that the cost estimates coming out of these studies (TIAX and DTI) include all the same elements as those coming out of the H_2 infrastructure side (e.g., H2A). For example, H2A has permitting costs, stranded asset costs, and assumed return-on-investments, none of which are in this study. DOE should put some effort into identifying some of these differences.
- Some stack assumptions require explanation.
- Greater depth needed for understanding the possibility of supply chain sensitivity and choice of bipolar plate.

Specific recommendations and additions or deletions to the work scope

- Revisit expediency of factoring in costs and benefits of Pt recycling, taking into account new approaches for Pt recovery that might make it more effective to start recycling at lower volumes.
- Include cost of battery, if you see this as a BOP component.
- Include grade of hybridization and therefore calculate optimized grade of hybridization.
- Do own analysis on cost of manufacturing membranes and bipolar plates.
- A question was asked about other volumes which is very important to the overall analysis and understanding of the potential market rollout. When doing these other volume analyses, it is also important to consider higher margins for the supply chain as they need to recover all of the investment dollars they have put in to these efforts. While that will slow the ramp of the pricing curve, it is more reasonable then just assuming the automakers will drive everyone to a 15% markup on cost.
- Harmonize the DTI and TIAX study assumptions because 1. the cost of Pt is different in the two studies. 2. the Pt loading is different in the two studies: 0.19 vs. 0.2 mg/cm^2. While this looks small, it makes a significant difference in the results because of the price (!) of Pt.
- Publish these results in a peer-reviewed journal. It would add a lot of credibility.

- Exploring greater variation of system components and plates (the non-MEA components) is recommended. If such exploration is already done, explanation should be given.
- Stack conditioning should be covered in the stack assembly section.
- The balance-of-stack components should be identified; the time required for assembly should be evaluated.

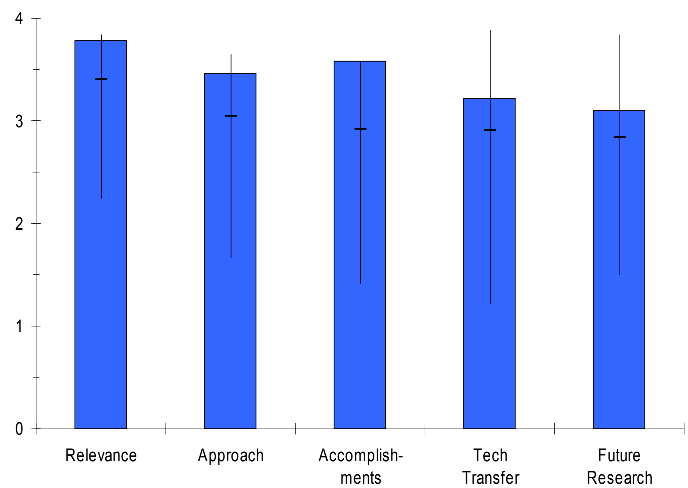
Project # FC-28: Mass Production Cost Estimation for Direct H_2 PEM Fuel Cell System for Automotive Applications

Brian James; DTI

Brief Summary of Project

The objectives of this project are to 1) identify the lowest cost system design and manufacturing methods for an 80 kW_e direct-H_2 automotive proton exchange membrane fuel cell (PEMFC) system based on three technology levels (current, 2010 and 2015 projected technology); 2) determine costs for these three technology level systems at five production rates (1,000, 30,000, 80,000, 130,000 and 500,000 vehicles per year); and 3) analyze, quantify and document impact of system performance on cost. The cost results will be used to guide future component development.

Overall Project Score: 3.5 (6 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.8** for its relevance to DOE objectives.

- Very relevant to the DOE Hydrogen Fuel Initiative and objectives.
- The results from this work will be very useful for fuel cell manufacturers targeting the automobile market.
- All the stack and systems components considered for this study are very relevant to the present state of technology.
- This project provides cost estimates for what PEM fuel cell production costs might be, and compares them to DOE cost targets.
- In some sense, this project might be viewed as "due diligence" by DOE to confirm that the Hydrogen Program has ultimate commercial viability.
- While providing some level of insight as to what cost reductions might be necessary to meet DOE cost targets, those insights are somewhat obvious (e.g., catalyst and GDL costs) and do not require such an intricate analysis. In other words, there is little need to price out (study in detail) the 2% and 3% costs when the major 20%, 30% and 40% costs are obvious (see slide #17).
- These types of studies are imperative to ensure that there is a reasonable path to meeting the cost targets of this significant application.
- These studies should also yield what particular improvements or technologies are required to meet the DOE targets.
- Few things are more relevant to DOE objectives than an understanding of fuel cell cost drivers.
- A detailed projected cost breakdown of present, 2010, and 2015 is very helpful in guiding future work.
- Even though much of the effort seems to duplicate the TIAX study, it provides valuable additional insight.
- In general, the task of estimating fuel cell system costs is highly relevant to DOE targets.
- This cost study adds to its relevance by identifying a matrix of technology levels versus expected volume.
- There is just one failing with regard to relevance – the scope of the project is limited to describing catalyst application techniques that will almost certainly be obsolete by the time of fuel cell vehicle commercialization (assuming all other targets remain relevant and that fuel cell vehicle strategy has not changed).
- Extremely important to do long-term DFMA cost estimates of the fuel cell system for the DOE's knowledge.
- Companies do their own studies, but these are proprietary, and DOE needs to have its own, independently generated estimates.

Question 2: Approach to performing the research and development

This project was rated **3.5** on its approach.

- DFMA approach is good.
- Systematic analysis of manufacturing costs for each step.
- Used the key technical targets from DOE targets to conduct the analysis.
- Used the current technology and component cost for FY2010 target analysis and used future technology and component cost for FY2015 analysis.
- Different technological approaches to manufacture same components were used in the cost analysis.
- Very practical approach of using present technology and not to anticipate the benefits of future technology.
- The presentation described the approach as "detailed, rigorous, and consistent." In fact, projections out to 2010 and 2015 cannot possibly be rigorous.
- The approach could be better described as "best guess."
- As was pointed out during the Q&A, and as confirmed by the presenter, the "best guess" methodology used combined the lowest cost options for various components even though they didn't work well together. That is, more realistic systems might pair a lowest cost option in one component with a more expensive option for another component.
- The presentation demonstrated a relatively good degree of research and detail, and a rather transparent process that spelled out the assumptions.
- The transparency of the methodology used here is highly appreciated.
- Looking at the impact of different volumes and different technologies is very good as well.
- Overall, a very good systematic and well-considered approach.
- Takes into account many posssible improvements in technology (higher temperature, reduced humidity, lower pressure, etc.) but does not provide for possible step-changes such as truly mass-manufactured, low catalyst loaded MEAs.
- Combines lowest cost components and processes, which may not be compatible for a complete and workable system.
- The approach is exactly what is needed – a matrix of volume versus technology levels.
- The use of proven and public manufacturing cost estimation techniques is detailed, specific, and adjustable.
- The approach allows for evaluation of competing technologies.
- The approach has one major failing: the mixture of technologies that are not amenable to each other (e.g., stamped metal plates with UTC-prescribed conditioning). Presenting alternatives (e.g., molded plates) helps to alleviate this concern.
- DTI uses extensive knowledge of fuel cell systems and design for manufacturing analysis (DFMA)
- Please investigate a larger variety of system design and material options that have different effects on costs.
- UTC's bipolar plate design is based on carbon and is self-humidifying. Steel plates may be cheaper in your long-term cost estimates, but could not achieve the same self-humidifying mechanism that UTC uses.
- The industrial reaction to this type of study (from Nissan and UTC) is that a series of very optimistic assumptions are made, which results in very low mass-produced costs. Is this the most useful approach for the industry? What about adding probabilities of success/ failure with one vs. another production design or material selection choices.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.6** based on accomplishments.

- Thorough analysis of the components and assembly process of stack system have been conducted.
- Individual component costs were analyzed carefully.
- The system cost estimate assuming 2015 technology is almost double the DOE 2015 target.
- Correctly identified the GDL cost impact and its importance.
- All the smaller aspects, such as stack conditioning time, were considered in the calculation.
- The calculation method is receptive of any future changes that may happen in technology or material front.

- The contractor performed well in their process research, manufacturing insight, and distillation of estimated costs.
- Good results for this point into the project.
- Gathering the input information and processing with known (and accepted) procedures to arrive at the results shown represents excellent technical accomplishments.
- The study provides the most detailed understanding we have thus far of what fuel cell costs will be in the future.
- Individual analyses of MEA components are highly detailed, although there is some room for improving the compatibility of these components.
- GDL manufacturing process should be validated with an industrial partner.
- Very thorough, technically knowledgeable analysis.
- UTC can not use stamp-printed steel bipolar plates with its MEA and system designs. One catalyst application technology may not work with another technology (like the electrolyte).

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.2** for technology transfer and collaboration.

- The data will be available to all fuel cell manufacturers.
- Significant input has been taken from different stack and fuel cell component manufacturers.
- Ongoing open relationship with fuel cell manufacturers will help in developing robost cost analysis method.
- The model will be shared with DOE, which eventually will be shared with all DOE partners.
- By its nature, this project requires extensive collaboration with industry in the research phase, in order to obtain insight and data.
- The accumulated data and conclusions of this project would be best reviewed by opening them to validation by all stakeholders (i.e., as part of the formal process).
- Claim that they have interacted with many suppliers and OEMS, but no list was provided. Hopefully, a complete list of contacts will be included in the written report, so that one can see if key parties are being consulted.
- While there was a lot of input from industry, there didn't seem to be much true collaboration.
- While collaborations exist for the study to be produced, there are specific areas where collaboration could help. GDL production is one example.
- There is too much reliance upon patents. Patent holders should be contacted in order to understand what is really described in the patent and whether the technology in question is applicable to the assumptions of the study.
- Collaborated with the Fuel Cell Tech Team and others extensively (slide 2).
- Tremendous amount of work trying to understand sensitive information from a host of industrial participants.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.1** for proposed future work.

- Low cost non-platinum catalysts will be considered.
- Annual updates will capture any new changes in material cost or process cost.
- Factors for any change in technology and material cost will be updated.
- The PI proposes to better cover some areas (e.g., non-precious metal catalysts, bipolar plate passivation).
- The PI proposes to use the analysis to date as a starting point to see how costs might be driven down.
- Notwithstanding the above, future research is of limited relevance to the overall program because its major conclusions would still be obvious and it would be further refining estimates of mere 2% and 3% cost components. That is, DOE effort would be better spent on overcoming barriers in its technical program.
- Good plan, but I would also recommend analyzing what subsidies would be required (to make FCVs reasonably cost competitive) under different adoption-rate scenarios. DOE should have some idea of the subsidies required to cross the "valley of death." These subsidies may be shared by industry and the government, but some order-of-magnitude estimates would be useful here. Additionally, one could include the impact of early-market volumes (non-automotive).
- The only future work mentioned was possible annual updating of results until 2011.

- Annual updating is likely important but it seems that fundamental changes in some models might be necessary to keep up with potential changes in the "best"system design , major materials, or manufacturing processes.
- The need to explore alternative fabrication techniques and to refine the BOP costs is shown and is well understood by DTI.
- There is considerable refinement that DTI can bring to other details of the technology. The reliance on patents should be replaced by further collaboration with technology developers.
- Please add probabilities of success or failure with one technology, process, or materials choice vs. another.
- Please show cost estimate final results based on carbon bipolar plates as well, not just steel.

Strengths and weaknesses

Strengths
- Very practical consideration of all the component, assembly and manufacturing costs.
- Comparisons of present (FY2006) and future (FY2010, FY2015) are very realistic.
- Good comparison of present and future component/assembly costs.
- The project satisfies some measure of "due diligence" in estimating the commercial viability of the research program (e.g., by estimating costs and comparing them to DOE targets).
- The project provides some measure of insight as to the major costs of a fuel cell system, and hence where the greatest opportunites for cost reduction might be.
- The project demonstrates a good level of performance in research, analysis, and transparency.
- Transparancy of the methods and assumptions used.
- Looking at the cost at different annual volumes.
- Well organized.
- Well executed.
- Important area of study.
- Systematic approach.
- Incorporation of competing technologies in evaluation.
- Detailed analysis of each stack and system component.
- Literature search.
- Cost estimation techniques.
- Knowledge of PI and his team on design for manufacuturing analysis and fuel cell system design.
- Highly detailed and transparent study.

Weaknesses
- The assumptions on perfect integration of the best products of different component technologies is not a good approach.
- This project has limited impact because it generates little new qualitative information (as opposed to generating quantitative estimates for that which was previous known qualitatively) that would affect management decisions on the course of the research program.
- Elevation of educated guesswork to "rigor."
- The learning curve for assembly costs appears to be unbelievably flat (e.g., hardly any change in system assembly cost going from 1,000 to 500,000 units per year is not realistic). Some "learning curve" for assembly costs should be considered. Realistically, manufacturing efficiencies are typically learned with experience (i.e., one's idea of how to make 500,000 per year today is probably wrong).
- It seems too tied to predetermined configurations and processes that don't necessarily "mesh."
- A combination of the least costly components and processes may or may not ever represent a workable system.
- Lack of compatibility of different technologies.
- Greater need for industrial collaboration.
- Different scenario analyses of different materials usage were not investigated. For example, only two designs assumed – either carbon OR steel used for bipolar plates – this was the only scenario variation considered for the design.
- No change in assembly costs between 30,000 and half a million – robotic assembly assumed for both – realistic?
- What is the differentiating feature of this DTI study compared with DTI's other DFMA stack studies?

Specific recommendations and additions or deletions to the work scope

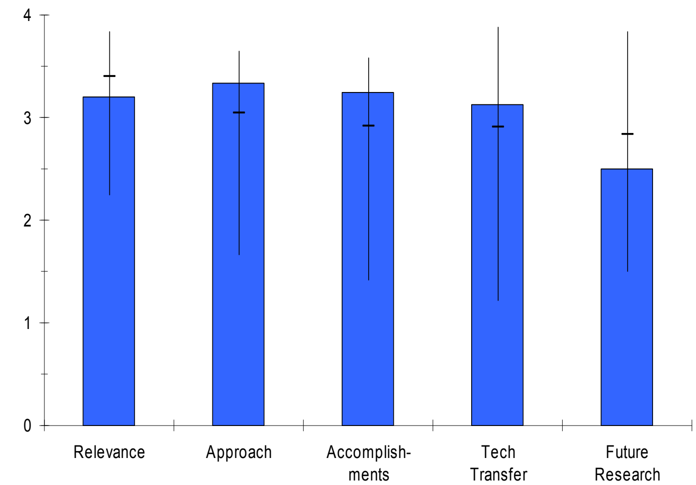
- Components from a working stack should be considered for the study to reflect the actual manufacturing cost.
- Components, such as membrane, GDL, catalyst etc., from different sources should be factored in the calculation to assess the practicality of the cost calculations.
- Consider adding some flexibility to the configuration and processes.
- Evaluate alternative catalyst application technologies including catalyst materials with alternative supports beyond high surface area carbon. Even though this is intended to be the assignment of the TIAX study, the TIAX study does not contain the approach and the rigor that DTI shows.
- Heightened contact with industry.
- DOE should not only allocate more funding for these kinds of studies, but also require industrial participants that it funds to provide data, advice, and feedback on these kinds of studies.
- More scenario analysis within the study – different costs of different design pathways.
- Make the models accessible in the Macro Systems Model so that industrial participants can do scenario analyses of different designs they may develop. For example, an industrial participant should be able to use the model to see the financial difference between using 1) a platinum-based catalyst and 2) a platinum-alloy based catalyst.

Project # FC-29: Platinum Recycling Technology Development
Stephen Grot; Ion Power, Inc.

Brief Summary of Project

The objectives of this project are to 1) assist the DOE to demonstrate a cost effective and environmentally friendly recovery and re-use technology for platinum group metal (PGM) containing materials used in fuel cell systems and 2) to use new processes that can also separate and recover valuable ionomer materials. DOE 2010 targets for membrane costs indicate membrane has value equal to the PGM. To achieve the project objectives, solvents will be used to “dissolve” ionomer and physically separate catalyst from ionomer solution in 1-5 sq. meter batch sizes. A best attempt to re-manufacture catalyst coated membranes with recovered materials will be made. Additionally, failure modes of membrane electrode assembly (MEA) materials used in fuel cells will be learned.

Overall Project Score: 3.1 (4 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.2** for its relevance to DOE objectives.

- Pt recovery is an important aspect of the overall fuel cell life cycle - it addresses both environmental issues and important cost issues that could ultimately impact the net costs of fuel cell systems. This project addresses important DOE goals, targets and objectives.
- Nafion recovery is not critical for meeting DOE objectives.
- Value of Pt recovery to the DOE program in unclear.
- Remaking Nafion into membranes is not critical for meeting DOE objectives - may be more expnsive than making fresh material.
- High relevance to the success of PEM fuel cells.
- Recycle (reuse) of expensive materials (perfluorinated ionomer and PGM catalyst) should be incorporated in the fuel cell cost model.

Question 2: Approach to performing the research and development

This project was rated **3.3** on its approach.

- The project has focused on a solid technical approach which explores reclamation of both the PGM and the ionomer membrane material.
- The PI of this project clearly understands the problem and has effectively structured the research program to addresss the DOE goals in this area and has identified and assessed risks involved in at least three potential solutions of the problem.
- Batch process seems reasonable to recover Nafion.
- Centrifuge shows good Pt recovery.
- May have difficulty when working with unitized assemblies.
- Technique may only be applcable for Nafion.
- Both catylst and ionomers are taken into account.
- Don't see a reason for looking after MEA failure modes in point of view recycling of the components.
- Important to analyze the limits of separation technologies.

- Also important to calculate the value of the recycled materials.
- Need to identify material specifcation to be reused (application) and clarify technical metric and criteria for success of this process.
- Need to pursue cost analysis to identify economical model of this recycle process.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.3** based on accomplishments.

- Excellent progress has been made to date - the project has demonstrated a high degree of PGM recovery and has also shown that Nafion membrane material can also be separated and recovered, although "enrichment" will be required to fully reuse the membrane material.
- Some scale-up of the process has been demonstrated.
- It was not clear that economic analysis of the proposed reclamation process has been conducted with the subsequent impact on fuel cell life cycle costs.
- Demonstrated scale-up of Pt recovery process - lost recovery.
- Recovered Nafion not in form suitable for recasting into membranes.
- No progess shown on understanding duarbility issues of MEAs.
- Good progress in scaling up the process.
- EOL Nafion similiar to BOL Nafion, great result for recycling method.
- Not only the recycling process itself is reviewed, also the cost and the energy the process needs.
- Propose only 2% loss in catalyst recycling.
- Progress was shown, however, need to clarify metric and criteria for this process success. Recycled material specification should be identified to develop metric and criteria.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.1** for technology transfer and collaboration.

- A number of collaborations were reported – apparently the collaborators provided important guidance and direction to the PI – it seems that most of the work was done in-house, however Delaware State and DuPont have, or will, play important roles in the execution of the work.
- Plans to work with DuPont on Nafion recasting, but nothing shown.
- Excellent partnerships between institutes and industry.
- Good collaboration to collect used materials.
- Industry collaboration is recommended to develop material reissue application and identify material specifications for these applications.
- Also, industry collaboration will be benefit for process scale-up.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.5** for proposed future work.

- Given the degree of completion (reported to be 70% complete) of this project, the future plans appear to be reasonable. It will be important to complete the remaining project tasks to assess fully the potential of the recovery process.
- Increasing collaboration with DuPont on Nafion film reprocessing not recommended.
- Investigating potential for use of recycled Nafion not recommended.
- No plans shown for improved Pt recovery process.
- No work on alloys is planned.
- What about reinforced membranes?
- Hydrocarbon membranes?

Strengths and weaknesses

Strengths
- Developed scaled-up process for Pt recovery.
- Interactions with stack suppliers as well as component suppliers.
- Development of IP to make the Nafion solution less dilute.
- Membrane material handling.

Weaknesses
- Too much focus on Nafion recovery – likely low value effort.

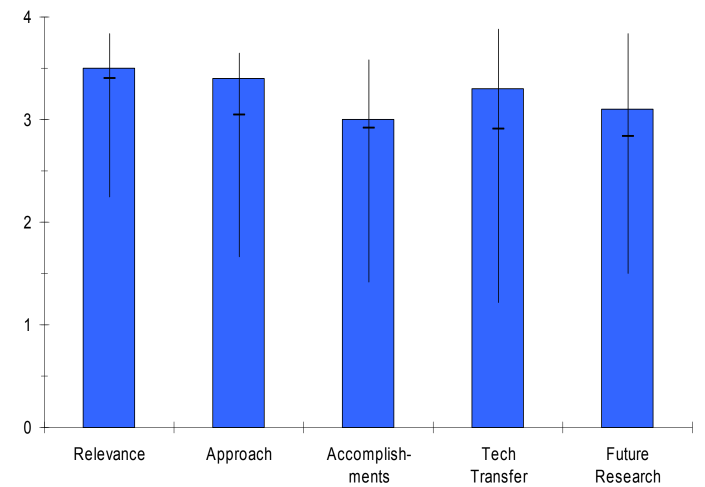
Specific recommendations and additions or deletions to the work scope

- It is important to complete at least a preliminary economic analysis of the proposed project.
- Investigate how recovery process must me done for a unitized assembly including seals, gaskets, adhesives, etc.
- Do economic analysis on value of recovering Nafion.
- Assuming Nafion recovery is not economically viable, focus on Pt recovery and stop work on Nafion recovery.
- Also work on alloy recycling.
- More study for application of recycled material is needed. Develop metric and criteria for process target.
- Develop cost model to be incorporated into fuel cell cost model.
- Industry collaboration for process scale-up approach.

Project # FC-30: Platinum Group Metal Recycling Technology Development
Larry Shore; BASF

Brief Summary of Project

Overall Project Score: 3.2 (5 Reviews Received)



The overall objective of this project is to develop and demonstrate a process for recycling of polymer electrolyte membrane (PEM) fuel cell membrane electrode assemblies (MEAs) without hydrogen fluoride (HF) emission. The objective for 2006-2007 is to re-design the process so that catalyst-coated membranes (CCMs) and Gas diffusion electrodes (GDEs) are processed together. Accomplished last year, a simple environmentally-benign, 'universal' process to recover Pt from fuel cell MEAs was developed with the following features: 1) no organic solvent required; 2) no need for combustion; 3) removal of gas diffusion layer (GDL) from membrane no longer necessary; 4) applicable to both CCM and GDE architecture; and 5) high yield with base metal-alloyed cathode catalysts indicated.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

- Pt (PGM) recovery is an important aspect of the overall fuel cell life cycle – it addresses both environmental issues and important cost issues that could ultimately impact the net costs of fuel cell systems. This project addresses important DOE goals, targets, and objectives.
- Addresses the main barrier for fuel cells – cost.
- High relevance to the success of PEM fuel cells.
- Project is focused on DOE goal to reduce cost of fuel cells due to platinum recycling.
- Without Pt recycling, fuel cell costs will be prohibitive.

Question 2: Approach to performing the research and development

This project was rated **3.4** on its approach.

- A solid technical approach has been taken in this project which was exploratory in the initial stages.
- Several potential reclamation processes have been surveyed and elimanated.
- The PI of this project clearly understands the problem and has effectively structured the research program to addresss the DOE goals in this area and has identified and assessed risks involved in at least three potential solutions of the problem. It appears that the project has been focused on the approach that is most likely to succeed.
- Approach to develop a widely applicable (both GDE and CCM) and environmentally sound recycling process is the only approach that would make business sense. Have developed processes which work with future alloy catalysts.
- Good approach to process CCMs and GDEs together.
- It's fine for me that they are focusing mainly on the catalyst.
- Approach is well-thought and focused on environmental-friendly processes for platinum recovery.
- Team has considered many recycling options and is willing to discard those that seem to show little promise.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- Significant progress has been made to date - however there is much remaining to be done in this project which was reported to be 85% complete.
- It will be important to complete the economic analysis and prototype process demonstration - it is not clear that enough time is left to complete these important tasks.
- Have developed a recycling process which avoids combustion and eliminates organic solvents and does not require preremoval of GDL.
- Have developed a process which is applicable to GDE and CCMs.
- Have achieved >98% recovery of the Pt with both CCM and GDE.
- Established a simple process without organic solvent, etc. and that's important to reach the DOE goals.
- Combustion process seems to be not useful for alloys due to Ru loss.
- Significant progress toward identification of the the most efficient process to recycle both CCMs and MEAs.
- Environmently friendly process was identified.
- Encouraging that the GDL does not have to separated first from the membrane.
- Environmental impacts of acids chosen for leachate procedure should be addressed. There must be some waste streams from the leachate to deal with. While it is true that PI has stopped further consideration of the VaTech method and its evolution of HF, I question the waste liquids generated by the acid leaching procedure. Need to understand this better.
- What is the target for %Pt/precious metal recovery?

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.3** for technology transfer and collaboration.

- A number of collaborations were reported – apparently the collaborators provided important guidance and direction to the PI – it seems that most of the work was done in-house at BASF (with the possible exception of Virginia Tech which assisted in one of the discontinued recovery processes).
- Working with membrane, catalyst, and MEA manufacturers. All the needed players are involved.
- It would be useful to have a collaboration with membrane maufacturer.
- There is a long list of collaborators, but it is unclear what they have brought into project (except materials).
- Collaboration with Virginia Tech was mentioned, but it is not on the list of collaborators.
- Although the NRL catalyst was tested, ONR instead of NRL was mentioned during presentation.
- Should talk to fuel cell stack manufacturers as well. Some of the packaging plans may add to the costs of the proposed recycling system.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.1** for proposed future work.

- Given the degree of completion of this project, the future plans appear to be reasonable. It will be important to complete the remaining project tasks to assess fully the potential of the recovery process selected by the PI.
- Proposed work includes economic study which will be important. Scale-up and demonstration is planned.
- Important to do the process economic analysis.
- What is the impact of alterative catalyst structures/compositions on the chosen recycling procedure? What about the 3M alloy – will it work on that?

Strengths and weaknesses

Strengths
- Extensive knowledge of catalysts and recycling of them.
- Fast identification of non-promising processes followed by redirection of the project.

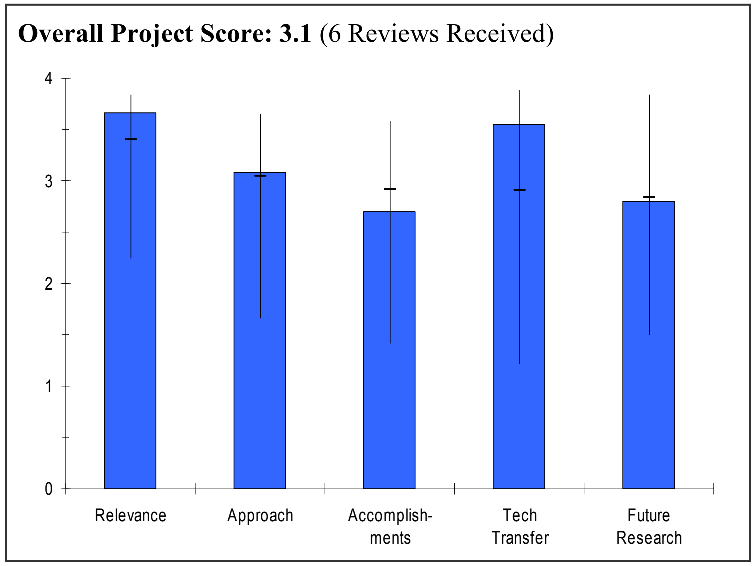
Weaknesses

- Deeper look at membranes needed.
- No cost analysis for cryo-grinding .
- Sources of MEAs, GDLs, and catalysts should be mentioned on slides.
- Should have a go/no-go decision point prior to proceeding to build recycling plant prototype.

Specific recommendations and additions or deletions to the work scope

- Environmental impacts of acids chosen for leachate procedure should be addressed.
- It is important to complete the economic analysis and prototype process demonstration.
- Include quantification of CO_2 emissions from energy usage in the process.

Project # FCP-01: Component Benchmarking
Tommy Rockward; LANL



Brief Summary of Project

The objectives of this project are to 1) provide technical assistance to fuel cell component and systems developers as directed by the DOE; 2) include testing of materials and participation in the further development and validation of a single cell test protocols with the U.S. Fuel Cell Council; and 3) provide technical assistance to the U.S. Council for Automotive Research (USCAR) and the USCAR/DOE Freedom Cooperative Automotive Research (FreedomCAR) Fuel Cell Technology Team. This assistance includes making technical experts available to the Tech Team as questions arise, focused single cell testing to support the development of targets and test protocols, and regular participation in working and review meetings.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.7** for its relevance to DOE objectives.

- Testing and training at LANL is valuable to material and component developers.
- The program addresses the testing of catalyst and development of test protocols to be used by PEM fuel cell developers. The benefit is achieving uniform procedures for the different fuel cell developers.
- This project nominally concerns various "benchmarking" activities in which test methods are developed and applied to determine the properties and performance of various fuel cell components and system attributes.
- This project provides outside access to experts and facilities at Los Alamos National Laboratory in support of various issues in fuel cell development, e.g., in a capacity similar to that of a consultant.
- LANL is gluing together many different components across industry and academia, both nationally and internationally. This is important work for keeping metrics/standards in fuel cells.
- This project is relevant to the DOE program and mission. The National Labs need to take a leadership role in aiding in technology transition. Part of the reason for their overall existence is to provide technical expertise to aid in the development of American industry and technology.
- LANL's work on fuel cells is on target regarding support for the H_2 Fuel Initiative.

Question 2: Approach to performing the research and development

This project was rated **3.1** on its approach.

- The protocols listed should be valuable to component developers.
- An extensive list of visitors to LANL was identified. It is not clear what topics were important to the visitors. The presentation should have provide some examples of the type of data exchange.
- Testing protocols were reviewed for the EU. The results of this review were not provided and it would help the reviewer if examples of the type of contributions were given.
- Los Alamos' strength in a "benchmarking" project should be in the use of its laboratory facilities as a competent and unbiased reference. But instead, the presentation emphasized the development of consensus test methods in various collaborative fora in which Los Alamos' contribution and impact was often unclear. That is, beyond

merely reviewing and commenting on proposed test protocols (within the technical capability of many industrial participants), in what ways did Los Alamos provide solutions based on its unique resources?
- It was difficult to determine exactly what this project entails – exactly what resources were being made available (and how they were being utilized).
- The written poster indicates extensive involvement in many technical areas, but answers to questions seeking additional detail were not so detailed.
- Overall approach is very good and leverages LANL's years of expertise.
- Not really clear the role that LANL is playing in each role – for instance, in catalyst stability protocols, each company has a method and it's not clear how LANL is integrated with those other protocols and whether they have compared them.
- Participating in meetings, setting up workshops and tutorials, as well as working collaboratively with U.S. reseachers and industry are an important role the national labs need to fill.
- LANL has an understanding of fuel cell fundamentals second to none.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.7** based on accomplishments.

- LANL has had many visitors and given lots of talks.
- No information of test results given (not even numbers of samples evaluated).
- No experimental data were presented by the organization; the program appears to be advisory and not part of a testing effort.
- LANL participates as a member of a team on the USFCC Durablility Protocols. It appears they reviewed the protocols but did not contribute to their development. With LANL's experience, I would expect that they would lead in the development of protocols and provide experimental data.
- The presentation lacked data showing results of benchmarking exercises. For example, in a "round robin" type of test one would normally show the different results from different testing laboratories (coded for anonymity) on the same object. In performance testing, one would show the measurements made on different samples (coded for anonymity) made by a single reference laboratory (or a group of well-coordinated reference laboratories).
- The presentation lacked description of specific technical acheivements attributable to Los Alamos that advanced the ability of industry to conduct testing. How did Los Alamos advance the art and science of performance testing in the laboratory (and what experimental data demonstrates such advances)?
- Not really clear if all 21 invited presentations can be claimed for this one program – 21 presentations seem to be from many LANL programs ($570K/yr).
- How much of leadership role is LANL playing?
- Obviously the technical accomplishments and progress from this program are largely proprietary. Nonetheless this program is interfacing with a wide variety of researchers and industry.
- Support for development of durability and catalyst durability protocols has been great.
- LANL could do more to speed up the development of test protocols for H_2 quality. We are still waiting for the results of the round robin baseline testing among LANL, University of HI, Clemson, and U Conn. H_2 quality testing is of critical importance to complete as soon as possible.
- Impurities in the H_2 are more problematic—whose responsibility are they?

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.6** for technology transfer and collaboration.

- LANL has lots of collaborators.
- Lack of data makes it impossible to deteremine value of these collaborations.
- The LANL fuel cell training class is planned but has not been held and may fit under future work.
- A long list of visitors is provided: LANL could provide a list of the information they transferred as part of a collaboration and this would be helpful for the reviewer and maintain a record of LANL's achievements.

- LANL reports they worked on a proprietary catalyst, but it was not clear if this was for a outside party that developed the catalyst or whether the proprietary catalyst was developed by LANL.
- The presentation contains an impressive list of collaborators, covering three slides, and presentations made, covering two slides.
- The extensive list of purported collaborators is disproportionate to the technical work described on the subsequent slides, in which principle interactions appear to be discussion participation within large consensus groups.
- The number of collaborations is truly astonishing!
- To ensure the best use of this program, the PI needs to take additional steps to ensure more researchers know that the program is available and the capabilities are available at LANL.
- Lots of training, tours, collaborations, presentations, etc.
- Excellent ties to USFCC, FreedomCAR and Fuel Partnership, and others.

<u>Question 5: Approach to and relevance of proposed future research</u>

This project was rated **2.8** for proposed future work.

- No future research was proposed.
- The future work is the training course.
- LANL will continue to advise the USFCC.
- LANL will continue to participate in the WG12.
- The presentation indicated that future activity would include participation in various round robin tests; otherwise it implied that the future would be more of the same.
- Overall very good plan to keep doing the same activities—presumably no program plans are listed.
- The future research is dependent on outside researchers and industry seeking out LANL and its resources.
- More a support project coordinated with USFCC and others, so future efforts are guided by a body outside LANL.

<u>Strengths and weaknesses</u>

<u>Strengths</u>
- Good test facilitites and personnel.
- LANL has a very strong reputation in fuel cell technology. The researchers and facilities at LANL should provide a strong basis for research and development.
- It is valuable to the fuel cell development and testing communities to have access to Los Alamos' facilities and expertise.
- The presentation indicates extensive outreach and networking with many potentially interested parties.
- LANL is providing a welcoming facility/resources to help unite measurement capabilities within the fuel cell community.
- Outreach to researchers and industry is an important component of the National Lab mission. These types of efforts need to be given additional resources.
- Vast collaboration network.
- Community education on fuel cells. The tutorials that LANL puts on are useful to train new people.
- Detailed understanding of fuel cell fundamentals.

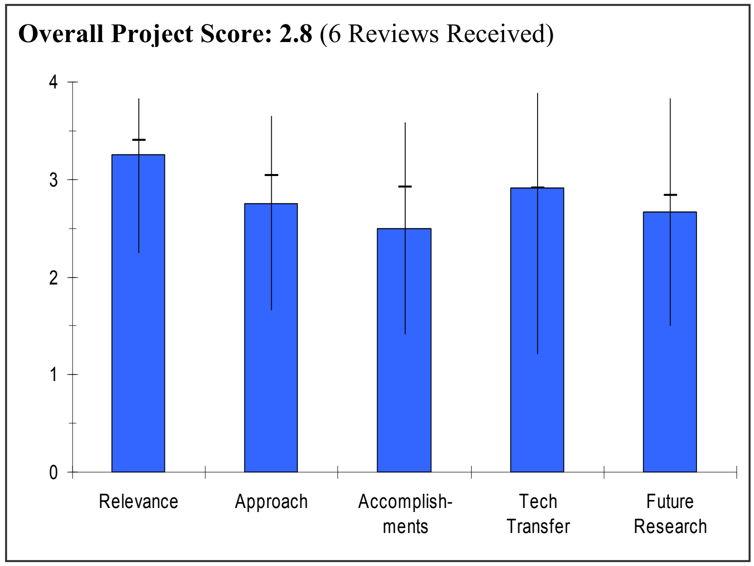
<u>Weaknesses</u>
- Lack of any statistical information on test reproducibility.
- Very little data were made available. The project is conducting reviews but little evidence of experimental activity is given.
- I think the presentation was weaker than the actual activities at LANL. A better description of the experimental activity should be provided.
- The presentation had undue emphasis on paper exercises (i.e., "review and comment") that did not utilize Los Alamos' laboratory facilities and other technical strengths (e.g., those not otherwise available in private industry).

- The presentation lacked experimental data providing technical justification for recommendations or decisions made in establishing testing protocols.
- LANL has a small amount of "not invented here" symptoms and they may want to update SOME of their methods, or at least validate their traditional methods against emerging ones.
- Additional advertising of upcoming workshops/events needs to occur. This program also needs to do a better job of communicating the capabilities that are available.
- Lacks sense of urgency.

Specific recommendations and additions or deletions to the work scope

- Show data for non-confidential materials.
- Do a statistical analysis of durability test results.
- Draw some conclusions from the data.
- At the very least, list the number of samples tested for each protocol. Then maybe a proper evaluation can be made.
- Increase the disclosure of data and information. The lack of reporting does not provide the fuel cell community with helpful information.
- This project had a 2003 start, yet the "Objectives" describe general areas of activity that the project "is expected" to entail. This project should be of sufficient maturity that the PIs should be able to articulate short and specific objectives that indicate exactly how they intend to (1) apply the technical strengths of Los Alamos to advance and to add value to the testing efforts otherwise being organized by the community, and (2) proactively use benchmark testing as a tool for advancing DOE program goals (that is, its role as a means rather than as an end).
- This program should definitely be continued as it is of broad service.
- The project needs to investigate new routes to advertise its existence.
- Recommend putting significant resources and timeline commitments on the impurities work. It seems to be moving too slowly.

Project # FCP-04: Kettering University Fuel Cell Project
Joel Berry; Kettering University



Brief Summary of Project

The overall objectives of this project are to 1) develop novel proton exchange membranes (PEM) for fuel cells and 2) develop a computational fluid dynamics (CFD) porous flow model for PEM fuel cells for improved water and thermal management. The objective for 2006 was to develop a low-cost, high performance membrane that includes experimental testing and performance validation.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

- The relevance of this particular appoach to the DOE objectives was not clearly stated.
- The project is highly relevant to the DOE's objectives and supports the President's Hydrogen Fuel Initative.
- The topic of the project fully supports the DOE RD&D plan.
- This project involves development of new polymeric membrane materials that prospectively might have superior properties.
- Though not yet reported, this project involves development of a new computer model (computational fluid dynamics) for the multiphase analysis of water and its vapor flowing through a fuel cell.
- Good effort that addresses DOE goals for membrane cost and performance.
- Project appears to be similar to research done by others.

Question 2: Approach to performing the research and development

This project was rated **2.8** on its approach.

- A rationale was not given for the choice of polymers and why these particular polymers will improve the membrane properties relative to Nafion.
- The method used for detemining proton conductivity, diffusion of protons detemined by pH change of aqueous solutions in contact with the membrane, is not relevant to fuel cell conditions.
- The technical approach for the program is good. The tasks are clearly presented.
- The testing setup for measuring the membrane proton exchange capacity is questionable because the membrane diffusion capability due to acidic concentration (pH) difference across the membrane is not an indication of its ionic conductivity. Instead, an electric circuit should be established such that protons crossing through the membrane is assured and the membrane ionic conductivity is appropriately measured.
- The membrane dimensional change in the x, y, and z directions, due to water uptake, should be determined with a relatively accurate non-contact measuring technique that utilizes optical or laser methods.
- The project is technically feasible.
- Commericially interesting membrane materials should also be judged on their chemical stability, their ability to bind and stabilize dispersed catalyst, the temperature range of their operation (e.g., to run hot to avoid CO poisoning of the catalyst), etc.
- The presentation did not propose that membrane conductivity is a limiting factor for fuel cell design. The electrochemical reaction at the cathode is generally regarded as the rate-limiting step.

- Increasing the conductivity of the membrane could perhaps lead to smaller fuel cells of equal power (e.g., higher power density), but only to the extent that protons crossing the membrane could react more quickly with the oxygen.
- Decreased cost is also cited as an advantage of the new membrane material, but no data is provided on either (1) prospective costs of the traditional and prospective membrane materials, or (2) the extent to which the cost of the membrane might influence overall fuel cell system costs.
- Innovative approach that leverages collaborator expertise to develop inexpensive membrane technology.
- Approach provides highly flexible platform for continued improvements using broad range of previously developed and/or new polymer chemistries.
- Though project claims to be addressing manufacturing costs, it is not clear how this is/will be addressed.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.5** based on accomplishments.

- Technical progress has been slow considering the funding level and that this is a two-year project.
- No results presented for the CFD modeling effort.
- The project was started July 2006. It is too early to make a judgement for technical accomplishments at this time. However, the project progress is good.
- The project is eleven months in progress with no evidence that supports the accomplishments as indicated by the PI: Task 2: Chemical modification – 80% completed, Task 3: Thermal stability and Water Management – 70% completed, Task 4: CFD Multi-phase model for PEM fuel cells – 40% completed.
- The presentation showed an impressive amount of data for a project of such maturity and level-of-effort.
- Large number of materials already screened, and several of the most promising are undergoing additional evaluation.
- Need to evaluate membranes at temperatures above 60°C.
- Significant progress in developing the theory and correlating it to their experimental results, at least for the more promising materials for which data was shown.
- The project claims to have discovered an "advanced" membrane manufacturing procedure; it is not described.
- Should show clearly the alignment of progress to technical targets.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.9** for technology transfer and collaboration.

- The inclusion of a catalyst company and a polymer company on the team is excellent. It is unclear, however, what participation these team members have thus far.
- The project was started July 2006. It is too early to transfer technology to industry at this time.
- Collaboration with two industries namely, Bei Tech and Umicore Fuel Cells were mentioned by the PI.
- The PIs collaborate with a German fuel cell manufacturer and a minor player in polymer membranes.
- Project strongly leverages expertise and prior technology demonstrations of the two identified collaborators.
- Strong working relationship with both collaborators, who continue to make valuable contributions to the program.
- Bei Tech and Umicore are mentioned as partners, but their roles are not clear.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.7** for proposed future work.

- Without full characterization of the materials developed thus far, it is premature to state that the future research should include improvements on the membrane properties (e.g., cross-linking). The first step in future work should be full characterization of the existing materials to determine if they hold any promise.
- Based on the presentation information, the future research work is clearly presented and technical approaches are reasonable.

- Good plan for the proposed future research work.
- Future research is described as, "seek answers by identifying factors limiting PEM fuel cell performance". Better focus is required both on general grounds and specifically because such a broad scope would require an extensive technical capability that the PIs do not have.
- The PIs plan to integrate their new membrane material into a working fuel cell and to measure its performance, a natural and appropriate extension of work completed to date. However, it is still not clear how this new material would advance the state-of-the-art.
- Very ambitious based on FY08 funding level.
- While the future plans for this project may lead to some additional knowledge being gained, these plans should focus more on overcoming barriers.

Strengths and weaknesses

Strengths
- The approach to membrane development may have some promise, but this needs to be demonstrated with the correct characterization techniques.
- The PI and co-Pi have good R&D experience for polymer membrane electrolyte chemistry.
- Good overall objectives that are complemented by well planned future research work.
- The quantity of experimental work completed to date is impressive for a project of this scale.
- Good theoretical and experimental research that is making good progress toward DOE goals.

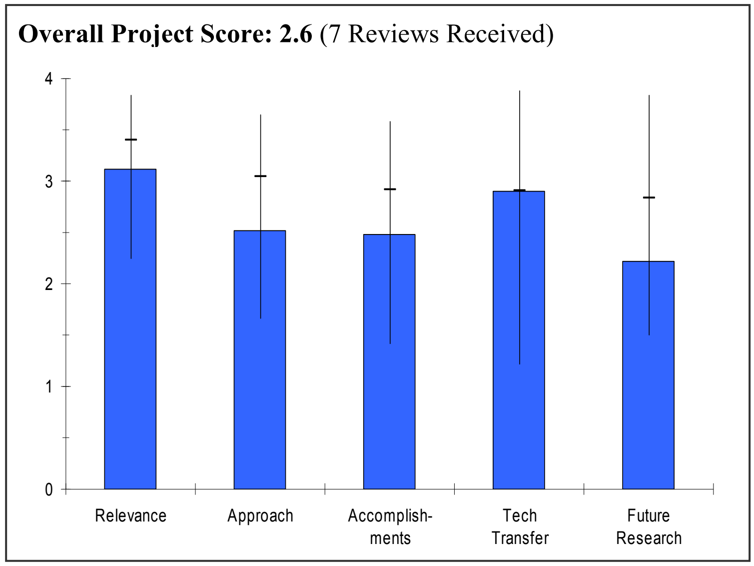
Weaknesses
- Lack of characterization of the polymers. If Kettering does not have the correct equipment for evaluation of the membrane properties, then they should utilize the capabilities of their stated partners or request help from either BekkTech or the high temperature membrane project coordinator, the University of Central Florida.
- Improvement in the measuring methods and techniques for the proton exchange capacity and membrane dimensions change due to water uptake is necessary. The project's rate of progress should increase to match the project two year duration plan.
- It's not clear what hypothesis the PI is trying to test or what specific technical barrier the PI is trying to overcome.
- Indicated that they had applied for a follow-on program, but could not articulate what they expected to demonstrate by the end of the current effort and what the focus of the follow-on program would be. Essentially said "just further exploration".
- Difficult to assess the extent of Edisonian versus good fundamental research since the process is proprietary. Makes it difficult to determine at what point membranes from this effort should transition.
- It is not clear that this project is doing anything unique.

Specific recommendations and additions or deletions to the work scope

- Increased interaction with the North American fuel cell industry is encouraged.
- Full membrane characterization and participation in DOE’s High Temperature Membrane Working Group for direction in correct membrane characterization protocol.
- This project just started the second year, project progress is good. No action is need at this time.
- Focus work on overcoming key barriers.

Project # FCP-08: University of South Carolina Fuel Cell Design Project
John Van Zee; University of South Carolina

Brief Summary of Project



The objective for Project 1 (non-carbon supported catalysts) includes developing novel materials (e.g., Nb-doped) for improved corrosion resistance and improved fuel cell components. The objective for Project 2 (hydrogen quality) is to develop a fundamental understanding of performance and durability losses induced by fuel contaminants. Project 3 (gaskets for PEMFCs) plans to develop a fundamental understanding of the degradation mechanisms of existing gaskets and the performance of improved materials. Finally, the objective for Project 4 (acid loss in polybenzimidazole (PBI)-type high temperature membranes) is to 1) develop a fundamental understanding of acid loss and acid transport mechanism and 2) predict performance and lifetime as a function of load cycle.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.1** for its relevance to DOE objectives.

- The project on hydrogen quality seems to be the most likely to have an impact by this team, while phosphoric acid research is not particularly compelling for the HFI.
- The primary work reported focuses more on modeling of flows, which can be related loosely but doesn't do much in terms of advancing any of the four research directions.
- The project is highly relevant to DOE's objectives and supports the President's Hydrogen Fuel Initative.
- The program addresses critical needs for the development and advancement of PEM technology.
- The hydrogen quality program is critical for achieving durability of the PEM fuel cell and assuring the cost of hydrogen is not excessively high.
- Gasket materials are critical for PEM fuel cells. Developing stable gaskets with high durability is a PEM fuel cell need.
- Acid loss is a critical problem of the PBI-type membrane and suggests that PBI is a matrix for holding phosphoric acid and not a membrane in the sense of perfluorinated sulfonic acid membrane. This is an issue that needs to be fully understood.
- The project is in complete agreement with the overall DOE objectives.
- A collection of disparate project areas that broadly support fuel cell development.
- The main projects of this program directly address the top three barriers of durability (catalyst supports, gaskets), performance(impurities) and cost (not sure how this is directed at reducing costs).
- The program also appears to cut across the transportation and stationary lines.
- Project appears to address some key barriers, but is not clear aligned to the Hydrogen vision.

Question 2: Approach to performing the research and development

This project was rated **2.5** on its approach.

- The approach of this group is very disconnected with no real synergy between the four different research areas.
- Within any given research area, the approach tends to be very vague on specifics and no progress has been made. More often than not, this degree of unorganization or lack of insight leads to poor progress.
- The technical approaches for the program are reasonable.

- The approach thoroughly analyzes the design of the conventional and optimized PEM fuel cell flowfields.
- From the data developed by this program, optimized designs of the flowfields and modeling of hydrogen purity effects for various PEM fuel cells will be possible.
- The degree to which the technical barriers are addressed is not fully described by the PI during the poster session and this could be attributed to the following: (1) The project just started two months ago and will continue for another 20 months. (2) The project consists of four subprograms that are not yet completely developed. (3) Most of the co-PIs of this rather large project did not participate in the poster session.
- The catalyst support corrosion issue directly addresses a critical limiting characteristic of current carbon supported catalysts.
- Determining the tolerance to hydrogen quality will presumeably directly impact the cost associated with hydrogen production, but not necessarily the cost of the MEAs or stack fabrication.
- The various projects appear to be unrelated from the information presented, and as such, for a two year program of this size, it is a concern that the degree of progress on any one will not be very deep.
- Too many sub-projects within this project.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.5** based on accomplishments.

- At this time, the only real progress is limited modeling on massively parallel flow channels that won't be used commercially. These are being used as the basis for doing impurity studies, but the models haven't been validated experimentally and its unlikely that they can be to the level that is necessary for the way they are hoped to be applied.
- No supporting/past work in this area has been presented to suggest that success should be expected from this work.
- The project was started Feburary 2007. It is too early to make a judgement for technical accomplishments.
- The modeling of the current density distributions in the conventional cell and the ideal cell provide a basis for understanding the overall performance of PEM fuel cells.
- The water modeling and hydrogen distribution will greatly help understanding the PEM fuel cell hydrogen quality experiments.
- The thermal modeling as a function of flowfield design will provide additional understanding with regard to the durability of the membrane. This is a bonus from this program and is not included in objectives.
- The project is showing a reasonable rate of progress.
- This project is just getting started and most of the work to date has focused largely in the area of modeling of cell current density distributions and temperature gradients. This type of work has been done many times before by many others, and there is really nothing new here.
- Better clarification should be presented as to how the MEA current density uniformity is related to hydrogen impurity – is the modelling done just because it can be or is there evidence to support it is a strong factor determining the stack response to fuel impurities?

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.9** for technology transfer and collaboration.

- Interaction with industry, centers/panels is important. This has not been demonstrated by the project yet or at least is unclear.
- Significantly more interaction with leaders in the field would significantly strengthen the project.
- Hard to rate technology transfer because program has just started up. Collaboration with Plug Power is a strong tech transfer effort.
- The detail and quality of the data reported at the review is outstanding.
- The project has identified Plug Power and 14 companies as collaborators, but there is little evidence of meaningful input or interaction so far.
- The opportunity for dissemination of results through the NSF IC/UCRC appears good. Direct interaction with Plug Power and probably UTC will also be beneficial.
- Though 14 companies are mentioned early in the presentation, there is no other explanation of collaboration in this project.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.2** for proposed future work.

- Plans to pursue sealants/gaskets and novel supports don't suggest that advancement of the state of the art is likely.
- Phosphoric acid loss/migration is not currently the limitation in the commercial deployment of these systems.
- The work on hydrogen quality is necessary, but the use of the model developed and parallel flow channels to evaluate impurities is unlikely to improve insight into hydrogen quality specifications.
- The task plan identifies the future work and the program is well-structured.
- The project did not clearly show any proposed future research work.
- The workplan is well-structured and carefully laid out.
- No slide was included to specifically state the future work.
- Since project has just started most work is still to come, so should consider splitting project into multiple projects with more focus.

Strengths and weaknesses

Strengths
- The PI has a good experience for the fuel cell R&D experience.
- Well-organized modeling effort.
- Top PEM researcher leading effort.
- The project interactions/collaborations include 14 Companies of NSF I/UCRC Center for Fuel Cells, DOE H_2 Quality Team and Plug Power partners.
- The project consists of four subprograms that are in complete agreement with the overall DOE objectives.
- Good modeling and interactions with partners.
- Project appears to be well-funded.

Weaknesses
- Little experience and no demonstrated performance in the area. Unlikely to supply much benefit to the program or advance the HFI.
- Based on the presentation information, only one PI for the program. The risk is high for the program. The program needs more co-PIs or coworkers to accomplish the projects.
- Program should address cross-flow flowfields.
- The project duration is too short for the large amount of work that needs to be accomplished.
- Very diverse topics which might stretch the resources too much to enable solid progress on any one project.
- PI is attempting to take on too many topics.

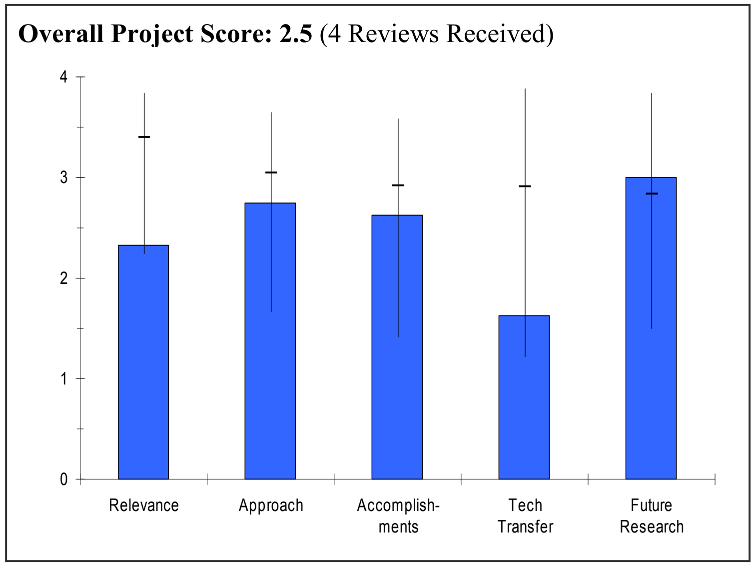
Specific recommendations and additions or deletions to the work scope

- Should focus effort on one key area.
- Hydrogen quality has needs that can be met by this team, but focusing on performance and diagnostics rather than modeling would be a better approach. Close coordination with others in the program in this area is necessary to make sure that meaningful contribution is added.
- Data supporting the potential of novel supports needs to be demonstrated to justify funding.
- Sealants/gaskets work needs to be guided by fuel cell developers or the studies may prove valueless.
- Phosphoric acid studies should be abandoned.
- The PI should add a co-worker to the project.
- Does DOE provide $1,655,000 for one PI only? The funding is too much for one PI (20 months). The funding for most university projects is ~$300K per year.
- Program should compare PBI fuel cell to phosphoric acid fuel cell using silicon carbide for matrix. Which of the two reduces the phosphoric acid vapor pressure and will extend the life of the fuel cell is a critical question.

Project # FCP-09: Development of a 5 kW Prototype Coal-based Fuel Cell
Steven Chuang; University of Akron

Brief Summary of Project

The overall objective for the project is to design a 5 kW prototype coal-based fuel cell and fabricate a small scale coal fuel cell system including coal injection and fly ash removal ports. The objective for 2007 is to fabricate and test a small scale coal fuel cell system. To achieve the objective, an improvement of the anode catalyst structure and the interface between electrode and membrane will be made. Refinement of the techniques for fabrication of the fuel cell assembly will also be needed. Interconnect materials for the coal-based fuel cell will be selected and tested.



Question 1: Relevance to overall DOE objectives

This project earned a score of **2.3** for its relevance to DOE objectives.

- It is not clear how a solid oxide fuel cell utilizing coal as a fuel is supporting the Hydrogen Fuel Initiative.
- Project to generate electricity directly from coal. In the long term, it is difficult to understand how this fits into the overall DOE program and what long term advantages it offers.
- Fuel cells uilizing coal directly could utilize the existing domestic coal resource on a small scale at high efficiency close to the load, saving line losses and enhancing reliability at the point of use. This is a strength of the topic.
- The lack of integration of the process with sequestration detracts from its benefits.
- Although this is not a hydrogen production topic, its electrical generation focus is consistent with DOE RD&D goals of high efficiency and domestic fuel use.
- To be more consistent with DOE RD&D goals of reduced CO_2 emissions, sequestration could be added to the process topic.
- Addresses DOE barriers for SOFC work.

Question 2: Approach to performing the research and development

This project was rated **2.8** on its approach.

- Given the low cell voltages and the lack of any emission control for the effluent of the SOFC, the approach should be justified by calculation of overall system efficiency and comparison with coal to electricity via combustion.
- The approach to improving cell performance on this high sulfur fuel is very good.
- Approach appeared to be very naïve. Very much an academic effort but without very much detail and very limited data to support the effort. There are many analytical/spectroscopic techniques that should be used in this program that are absent. One specific program goal was the removal of fly ash from the cell during operation. There was no indication that this technical objective is being pursued.
- Although the "fly ash" is supposed to not adhere to the anode, the "fly ash" removal methods were not successful in removing the "fly ash". This should remain a high priority.
- What will be done with the CO_2 emissions?

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.6** based on accomplishments.

- This is a very challenging project and the short-term performance on coal is impressive.
- Showed several graphs that indicate that a cell is capable of converting coal into electricity. Overall efficiency very low. No indication of potential cost or efficiency improvement.
- Current accomplishments include interconnect development, successful operation on coal, verification of loose "fly ash", and comparisons with other systems. These are significant accomplishments.
- The development of a "fly ash" removal method may be difficult. Without development of a "fly ash" removal method, the advantage of loose "fly ash" might not be utilized to its full potential value. This topic needs to be stressed in the near term.
- The current project scale is extremely small, compared to the project goal of 5 kW. Some assessment of the path to larger size demonstrations (and up to the project goal of 5 kW) could help to ensure that the project goals are met within the project contract terms. This is a suggestion for additional emphasis by the project manager.
- If the durability is proven out, the achievement of 750-800°C operation is a significant achievement.
- What is the overall efficiency of converting coal to electricity for THIS fuel cell? I saw some general statements, but they were all generic. What is the efficiency target for this system?

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **1.6** for technology transfer and collaboration.

- No outside interaction is evident.
- Did not appear to have any tech transfer opportunities or collaborations.
- Need to get some industrial partners if they ever hope to commercialize the system. Maybe GE?
- This is a university operating in a vacuum. The only real-world development tie is the Ohio Coal Development Office. Needs more collaboration.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- The proposed future research addresses the issues of taking the initially promising small-scale single cell results to the stage of demonstration of a stack.
- Beyond simple stating that the cell efficiency needs to be improved, there did not appear to a well defined future research plan. There were not details given even on the proposed path to higher efficiency.
- Future work planned is appropriate, with emphasis on the goals of the research.
- It is time to bring in a collaborator with industrial engineering expertise.

Strengths and weaknesses

Strengths

- Prior work is well documented and the current project builds upon prior experience. This is a strength of the project. The project tries to reduce the impact of "fly ash" on the fuel cell anode. This is a good goal and some progress has been made.
- The graphical evidence provided is helpful in understanding the technology topic.
- The PI is very knowledgeable about SOFCs and has identified what issues need to be addressed to demonstrate them.
- The project emphasizes the use of a domestic resource – coal – in a highly efficient and customer supportive way.
- The project builds on prior experience and work.
- The project has accomplished many of their goals.

Weaknesses

- Analysis of system efficiency and system design is missing. This type of analysis would illustrate if this approach for converting coal to electricity makes sense.
- The project could really benefit from some collaborations with the larger community capable of using a variety of spectroscopic techniques to understand the cell/material function and performance in this approach.
- The project could be improved by coordinating and fully integrating sequestration issues into the project and into the technology development process.
- The project size is very small now, compared to the goal of a 5-kW system.
- The project accomplishment, of showing that "fly ash" does not adhere to the anode, may be hard to take advantage of without an effective "fly ash" removal technique.
- System performance degradation, ostensably due to "fly ash" build-up, is probably too severe to allow use of this technology on a commercial scale. Degradation needs to be improved - ostensibly by implementing a "fly ash" removal method.
- System is optimized for a particular coal from Ohio. What about other coals? Will it work for them? Especially with different sulfur content.
- Need a plan for fly ash management.
- Need a partner with a business and scale-up focus. Otherwise, unanticipated problems in making a commercial product could doom the work to failure.

Specific recommendations and additions or deletions to the work scope

- Additional future work is suggested to fully include sequestration of CO_2.
- For coal resources to support the DOE RD&D goals of lower CO_2 emissions, this project must be integrated with sequestration. It is suggested that this integration be accomplished now, while the project is in progress, to ensure that the technology developed here is compatible with sequestration.
- The poster included several technologies, some of which were for comparison with the technology of interest. Although this is helpful for comparison, it may also be confusing to some readers. It is suggested that in the future, the comparisons be separated out to avoid confusion with the topic of interest.
- The project could be improved by making the graphs consistent in terms of scale and units.
- Without a successful "fly ash" removal method, the advantage of the "fly ash" not adhering to the anode could be lost. This should be a topic for future high priority work.
- Suggest system design and efficiency analysis.
- Project is quite specifically tied to Ohio's coal industry. Expand to the national interest and get away from only Ohio coal operation. Or, explain that Ohio coal (sulfur content, ash content, moisture, and all the rest) are similar to other coal sources—I think it is not.

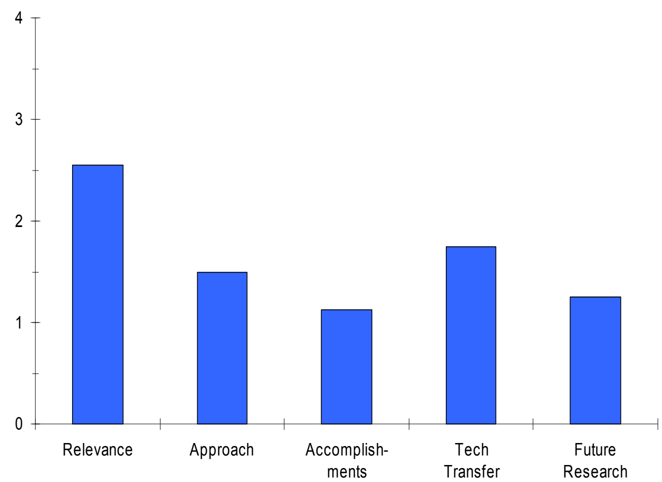
Project # CCP-01: Development of Advanced Manufacturing Technologies for Renewable Energy Applications

Charles Ryan; National Center for Manufacturing Sciences (NCMS)

Brief Summary of Project

The National Center for Manufacturing Sciences (NCMS) is working with the U.S. Department of Energy (DOE) and the private sector to identify and develop critical manufacturing technology assessments vital to the affordable manufacturing of hydrogen-powered systems. This project leverages technologies from other industrial sectors and works with the extensive industrial membership base of NCMS to do feasibility projects on those manufacturing technologies identified as key to reducing the cost of the targeted hydrogen-powered systems.

Overall Project Score: 1.6 (4 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **2.6** for its relevance to DOE objectives.

- Partner such as Millennium Cell needs to demonstrate their results from this funding. Partners such as Freudenburg/UTC/Cabot and DuPont may prove more fruitful.
- Manufacturing research and development is an essential component to achieving the cost targets for the PEM vehicle.
- The transition from laboratory to PEM vehicle production will be through several phases including portable and stationary fuel cells. The manufacturing efforts need to address these different applications.
- A broad base of manufacturing efforts will need to be developed to move the PEM technology forward and the program must structure itself for this diversity in manufacturing technology.
- Great titles for the eight projects: "low-cost," "high-reliability," "Manufacturing process," etc., but I could not begin to decipher what the individual projects were about or what they have accomplished. NO CONTENT in the poster.
- The field of manufacturing is highly significant and needs to be pursued and in general the topics sound good on the surface as they were presented. The actual individual programs vary from relevant (projects 1, 4, 7) to nearly irrelevant to the goals of the DOE program.

Question 2: Approach to performing the research and development

This project was rated **1.5** on its approach.

- It would be nice if there were some balance of plant components developers involved.
- The approach attempts to fund too many programs at levels not consistent with being able to complete the R&D effort.
- The approach has a limited prospect of success because the expertise in fuel cell technology at NCMS appears to be limited.
- The federal funding level was at $4.9 million for 2004 and 2005. It was not clear what the distribution of funding was to the eight projects.
- The presentation should identify what the funding levels and cost share levels are for these projects.

- Having NCMS get monies, then do basically their own solicitation for projects is not an effective way to generate projects that address R&D barriers.
- Low-Cost, High-Volume Manufacturing for PEMFC Power Plants seems to have a few useful aspects. LBNL looking at leachates on what might be called balance of plant could be useful, but there were not enough details to judge. And what is the impact of the leachates? Need better coordination with several fuel cell manufacturers to ensure relevance.
- Need to define targets (including cost and performance) for each of the eight projects.
- In many cases the technical barriers approached are not those where the material science is leading.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **1.1** based on accomplishments.

- Not clear at all if all partners made any kind of real accomplishments towards a low cost system (real numbers, not percentages).
- Each of the projects report varied levels of success.
- The interview with NCMS's representative was not very productive as he referred me to the individual companies who were not represented.
- It was not clear what part of the activities that were reported were covered by NCMS funding; e.g., the one-step process by Protonex was reported prior to the start of this project; March 2004.
- The "Low-Cost, High-Volume Manufacturing of PEM Fuel Cell Power Plants" did not report any results or participation by UTC Power. What was their contribution?
- Cabot has successfully completed an ATP program with NIST on ink-jet printing. What part of the NCMS program is different from the ATP program?
- Freudenberg and UTC Power have a separate DOE program for a low cost seal. How do these two programs differ? This should have been addressed by NCMS.
- High-Rate Mfg of Carbon Composite Tanks. The OEMs are moving to 70MPa tanks. This work is for 35 MPa tanks. Is the work relevant to 70 MPa? Objective of 6 min cycle time might be relevant, but can they do it for 70MPa tanks?
- Low-Cost, High Volume Ink-Jet. No cost data or estimates, despite the title.
- Low-Cost, High Reliability Seals. No cost data or estimates, despite the title.
- Develop Low Cost MEA3. No cost data or estimates, despite the title.
- Low-Cost, High Volume Manufacturing for PEMFC. No cost data or estimates, despite the title.
- Affordable, High-Rate Manufacturing of Carbon Composite Tanks. No cost data or estimates, despite the title.
- Little valuable progress as far as can be determined since 2004. For example the potentially valuable tank wrapping program still has essentially only concepts to show. The cartridge fuel project has made some progress but it is of limited application, none the less they have apparently made progress though the 1 use concept is clearly unfeasible in mass production. The Stack forming program beat its target but the target is not correlated to the DOE target (it is at about 1/2 current power density). No meaningful progress on testing and it is aimed at the wrong sort of tanks so any progress would likely have no impact on DOE targets and goals. Inkjet process has potential but not at all clear the right testing is being done to verify the results are meaningful to real MEAs. Sealing still not at a degree of progress that might be evaluated really. Project 8 has potential but unclear how good progress actually is.
- Above all there is no cost numbers given; that is what manufacturing lives and dies by.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **1.8** for technology transfer and collaboration.

- Some collaboration among industry members per project. Very unclear if all the players in this program interact with each other.
- No technology transfer was reported. The program allows individual companies to develop technology and intellectual property without disclosing the technology. Based on technology transfer, the rating is 1.

- The collaborations were high with several teams formed to solve problems. Based on collaboration the rating should be 3.
- I am sure the results are helpful to the companies participating. Whether or not these projects are ever useful to anyone else is hard to judge if no data/results are ever presented at the reviews.
- Essentially individual programs operating in isolation

Question 5: Approach to and relevance of proposed future research

This project was rated **1.3** for proposed future work.

- None was presented.
- The presentation did not report future work for NCMS. The rating would have been higher had they reported future work.
- Individual projects were continuing.
- Because I saw virtually no proposed future research, I cannot comment on their proposed future research.
- Unclear exactly where this is going. In the cases where it is clear I can not see how it will actually advance storage because the work is aimed at things that are clear how to do, not where research is actually needed.

Strengths and weaknesses

Strengths
- A few good partners who are very capable of delivering a good product to support the fuel cell industry.
- Many of the companies are well established in the fuel cell arena and bring strength to the program.
- POTENTIAL collaboration network that NCMS brings to the table. I am not seeing it, though, in the implementation of these eight projects.

Weaknesses
- No real cost data to show the current cost of the system/process to know how much they are closer to a mass market product.
- Discussions with NCMS representative were not productive. Representatives from the companies should have participated.
- The presentation did not follow the guidelines provided by the DOE; no future work identified by NCMS.
- It not clear what value NCMS brings to the program since they appear to not be able to review the technical status of the projects.
- This NCMS "project" has been underway for a couple of years now. It is time to see results. They may have results for some of the eight projects, but we sure are not seeing any results or useful information at the Annual Reviews.
- Participants in all the other DOE projects underway manage to present real results and show progress at the Annual Reviews and at FreedomCAR and Fuel Partnership tech team meetings despite the constraints of showing only non-proprietary information. Why can't NCMS and the eight project partners do this???
- Should be required to develop targets for each of the eight projects, hopefully tied to DOE targets, and show progress towards those targets. Otherwise, impossible to judge the merit of the work.

Specific recommendations and additions or deletions to the work scope

- Real cost numbers should be published. 30% reduction in cost is meaningless unless the final cost is affordable by the customers.
- DOE should work with NCMS to get them more aligned to the reporting of results and following the DOE program guidelines.

- Manufacturing is an important aspect for PEM fuel cell advancement, but NCMS does not appear to have the expertise in fuel cells to directly participate. The expertise of NCMS should be improved.
- Cabot has successfully completed an ATP program with NIST on ink-jet printing. What part of the NCMS program is different from the ATP program?
- Freudenberg and UTC Power have a separate DOE program for a low cost seal. How do these two programs differ?
- I recommend that EACH project team (of which there are eight) be required to present their RESULTS at the next Annual Review. The current process is not working.
- The NDE testing project team should review their project with the Production/Delivery tech team if they have not already done so. Likewise, the Codes & Standards tech team might be interested in a report of progress. Again, though, they need to show some real data and results.

2007
Technology Validation
Summary of Annual Merit Review Technology Validation Subprogram

Summary of Reviewer Comments on Technology Validation Subprogram:

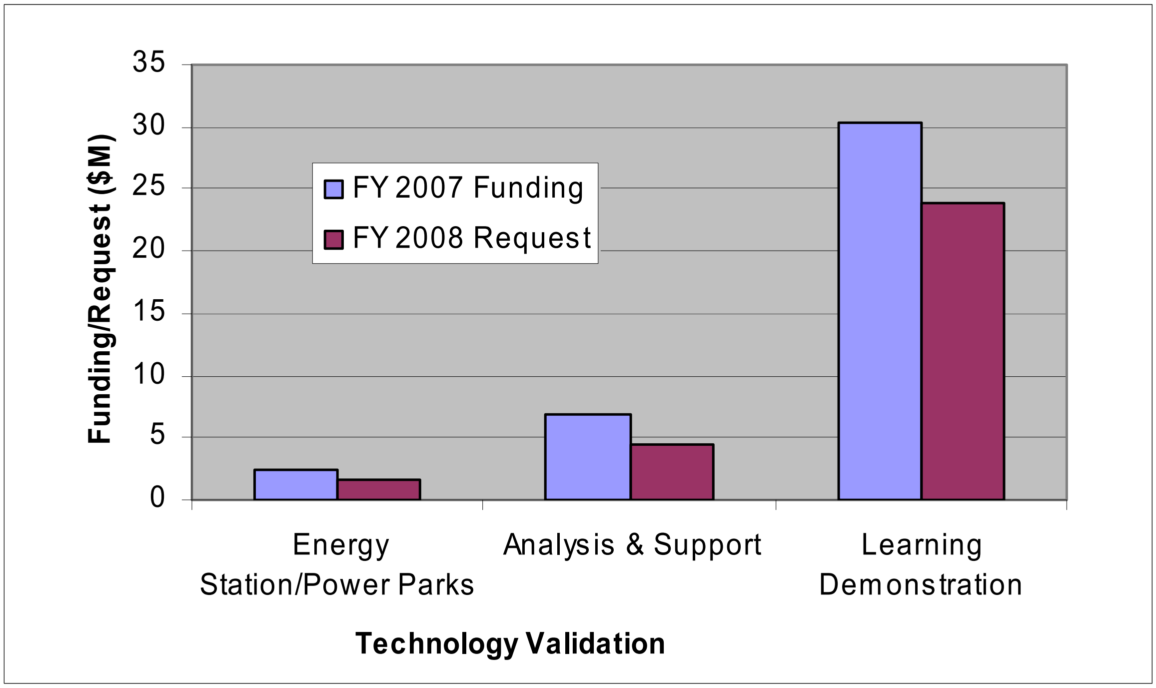
Reviewers think the learning demonstration project is an excellent match with DOE targets and the President's objectives. In addition, the learning demonstration is an important program that will provide a baseline of performance for today's PEM fuel cell powered vehicles. Gathering data on a number of vehicles in several locations and also collecting fleet experiences is important to understanding the true status of the technology in real-world applications. Good progress in getting the fueling stations operational. Several different locations with different climates are involved. Data collection is well done, focused and intelligent. The data collection and dissemination is exactly what DOE needs to have to maintain the proprietary data.

Reviewers thought that industry must open up its database and have more public disclosure because of the high profile industry and the government have given to hydrogen vehicles. More analysis on performance of the vehicle and the fuel cells would be helpful. Reviewers indicated there should be an increase in miles driven and the number of vehicles available so that stations can be more fully utilized and more information on potential improvements generated. If possible, some baseline comparisons with conventional technology in similar service would help show the progress toward commercialization.

The Integrated Hydrogen Energy Station project is excellent and very promising for very low cost hydrogen and electricity production. The greatest value of this project will come from an installed, working station generating real-world data. There should be an extended operational term with comprehensive data gathering covering efficiency, well-to-wheel emissions and energy use.

Technology Validation Funding by Technology:

The funding portfolio for Technology Validation stresses the continuation of the 6 year Learning Demonstration project as it enters its fourth year. Second generation vehicles began to be introduced in 2007 and data collection over the next few years will provide information on meeting 2009 fuel cell durability and vehicle range targets. A high temperature fuel cell Energy Station will be funded and constructed in 2008 followed by a year-long demonstration of the system. The FY2008 funding profile is subject to Congressional Appropriations.



Majority of Reviewer Comments and Recommendations:

The Reviewer scores for the Technology Validation Subprogram were on average slightly higher or similar with those of other subprograms (the maximum, minimum, and average scores for Technology Validation projects were 3.8, 2.9, and 3.4 respectively. These compare to the overall maximum, minimum, and average project scores of 3.8, 1.6, and 3.1, respectively. The Technology Validation project portfolio mainly includes the Learning Demonstration in the third year of the 6 year project. In addition, an Integrated Energy Station and cryo-compressed storage tank demonstration will be funded. The major recommendations by reviewers are presented below for each of the task areas. DOE will act on reviewer recommendations as appropriate for the overall Hydrogen Technology Validation effort.

- **Learning Demonstrations –** Project is important effort to demonstrate the feasibility of fuel cell vehicles and hydrogen infrastructure. More analysis should be included on the vehicle performance and the cost of delivered hydrogen.

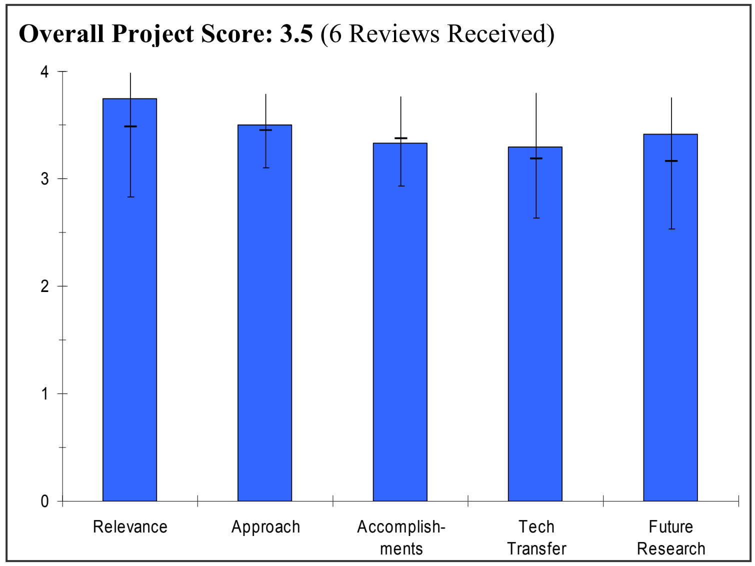
- **Energy Stations –** Extended operational term with comprehensive data gathering covering efficiency, well-to-wheel emissions and energy use. Work with project partners (or add partners) to fully test system capabilities by adding hydrogen vehicle fueling demonstration.

- **Storage –** A commercialization plan should be developed with suppliers. The project addresses DOE goals related to hydrogen storage aboard a vehicle.

- **Analyses –** The analyses of the Learning Demonstration should include information on lessons learned and benchmark this effort against European and Japanese initiatives.

Project # TV-01: Controlled Hydrogen Fleet and Infrastructure Demonstration and Validation Project
Klaus BonHoff; DaimlerChrysler

Brief Summary of Project



In this project, DaimlerChrysler deployed 30 Gen I fuel cell vehicles in three ecosystems to validate current status of: 1) Durability of fuel cell stack and system; 2) Range of operation with compressed H2; 3) Cost of H2 from various production methods; and 4) Performance degradation over life via dynamometer and on-road testing. All 30 vehicles were equipped with a customer friendly Fleet Data Acquisition (FDA) system that automatically collects statistically relevant data for submission to NREL as well as engineering analysis for technology improvement. To date, the vehicles have accumulated 130,000 miles and three driver perception surveys have been completed. Two refueling stations are in operation in Michigan (DTE and NextEnergy) with one planned for California. DaimlerChrysler, BP, DTE, and NextEnergy will also test emerging technology with the potential to meet DOE hydrogen cost target while evaluating emerging and renewable technologies to produce hydrogen and co-generation technologies to produce hydrogen and electricity. Data will be provided from Gen II vehicles under the same operating conditions as Gen I vehicles to compare technology maturity over the project duration.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.8** for its relevance to DOE objectives.

- The objectives were clearly stated and were consistent with DOE's MYPP.
- This is an important program that will provide a baseline of performance for today's PEM fuel cell powered vehicles.
- The difficulties establishing a hydrogen infrastructure will be established in this program.
- The project will provide data for planning of future projects by industry and the DOE.
- Directly relates to DOE goals
- Getting these fuel cell vehicle demonstrations on US highways, and doing that task correctly, is an essential step in the DOE hydrogen program.
- Very good, covers all important aspects.
- In spite of its high visibility, this project's value (especially per-dollar value) to advancing Hydrogen Initiative and bringing fuel cell technology closer to the market is not obvious.

Question 2: Approach to performing the research and development

This project was rated **3.5** on its approach.

- They use wireless data collection to ensure customer convenience.
- They need to raise public awareness better. This is on their radar screen to improve.
- 130 thousand miles driven.
- Three cities with good data displayed showing temperatures, different driving conditions, steep roads and stop-and-go traffic.
- Customer and perception study (49 participants) – most respondents felt safe driving the vehicles.

- The approach is well organized to obtain the technical data and the market data needed to resolve the many issues that will impact the introduction of PEM fuel cell vehicles.
- The combination of PEM fuel cell and hydrogen infrastructure in the same program properly identifies the critical technologies.
- The need for codes and standards is properly addressed in this program.
- Good approach but needs to expand variety of "customer's" needs to include full climate exposure i.e. parking and refueling.
- The program asks all the correct questions. Focus on customers and public interest is excellent.
- Good description of key parameters.
- Customer perception is good survey approach.
- Different climate testing is very good.
- Minimal technical content makes judging this approach difficult; based on available information, the approach does not appear to be particularly innovative.
- Stress on outreach and familiarizing average car buyers with fuel cell technology for automotive transportation is very useful.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.3** based on accomplishments.

- Completed a management plan within their company and for the public.
- Driving ranges were analyzed.
- They participated in 80 events with the vehicles. They also participated in many education events.
- Good infrastructure accomplishments in LAX, Michigan with DTE, and San Francisco.
- They have developed documentation on lessons learned with NextEnergy Hydrogen Fueling Stations.
- The operation in different climates is a critical part of the program and the data presented showed the climates but did not give the data for the vehicle operation. Was the vehicle operated in all the different climates?
- The program is progressing and developing the database for high velocity and stop-and-go driving.
- Fueling data demonstrates safe operation.
- Market data collection will provide future design and system characteristics.
- Good progress demonstrated.
- Data taken in areas with two different climates. Good job done to get training for safety and other governmental officials. Excellent data set collected that includes driving patterns and personal reactions to the vehicle driving experience. Excellent effort in education, informing the public. The lessons learned are also a very interesting and worthwhile data set.
- No discussion / results on key parameters used in the approach.
- The customer survey results are good. The pool size is too small.
- Fleet data summary is good – can be further quantified with useful information.
- No data on FC performance or range.
- Very little technical information makes judging progress very difficult.
- Interesting data collected in the customer perception and acceptance study.
- Little apparent improvement to the range.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.3** for technology transfer and collaboration.

- DTE Energy, BP and NextEnergy are business partners. Their interaction was not described very well. It is implicit that they work closely with their partners.
- Strong track record of working with government agencies, non-profit organizations and for-profit organizations.
- Outreach program providing education base for consumer and future consumers.
- Strong infrastructure is being developed in California. Infrastructure in Michigan appears to be focused around Detroit area and not the whole state.
- What about the rest of the country?

- How will this program address approval of facilities by local fire marshals?
- With a number of outside organizations involved, collaborations appear acceptable but need to include and expand to general public.
- Great team with fuel suppliers, regulators, customers, and other stakeholders.
- Very good activities and outreach events.
- 30 vehicles is a good target.
- Strong partners, seemingly well-coordinated effort.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.4** for proposed future work.

- They indicated that more miles and more data needed.
- They said they need to demonstrate refuelings for the mobile unit – yet they have already demonstrated 640 refuelings.
- Continue the site development for the Los Angeles Station. It is unclear if this is a new station.
- Well organized future work activities.
- Infrastructure work focused on California. Is the effort in Michigan finished?
- Exposure to climate extremes.
- Future plan is for more miles and more data, exactly what is needed. Moving 70 MPa tanks into the next program phase is an important task for this next effort.
- Good summary.
- It will be helpful to provide measurable qualitative goals to match with the approach.
- Much of the same – no surprises here.

Strengths and weaknesses

Strengths
- They have good data collection through a wireless data collection system which has little impact on the customer.
- They are sensitive to how the customer has reacted to driving the fuel cell vehicle and refueling the vehicle. Their perception survey provides essential feedback.
- Strong commitment to development and demonstration of technology.
- Good investment by industry to make program a success.
- "Customers" are limited to fleets (fire and police) climate exposure only during operation (not parking).
- Excellent project team. Solid base in first phase to build upon.
- Good outreach.
- FC strength of Ballard (though not emphasized/mentioned).
- Significant number of tested vehicles possibly allowing DaimlerChrysler for more reliable data collection and analysis of the strengths and weaknesses of the company's fuel cell car technology at its present state of development.

Weaknesses
- More information on the vehicle performance would be helpful.
- More analysis on performance of the vehicle and the fuel cells would be helpful.
- Data are not fully disclosed. Much of the effort looks like a press release and not technology validation.
- Industry must open up its database because of the high profile industry and the government has given to hydrogen vehicles.
- Expand customer base, widen public exposure and promotion, and add more economic evaluation.
- Provide info on utilization of refueling stations and the availability factors.
- Approach to go down to $3.00/gge not defined/evaluated
- Virtual absence of technical information.
- Without establishing a way of unobstructed flow of technical information, this and other technology validation projects have little value to component manufacturers.

- Very high project cost, possibly at an expense of underfunding the development of critical system components (stack components in particular).

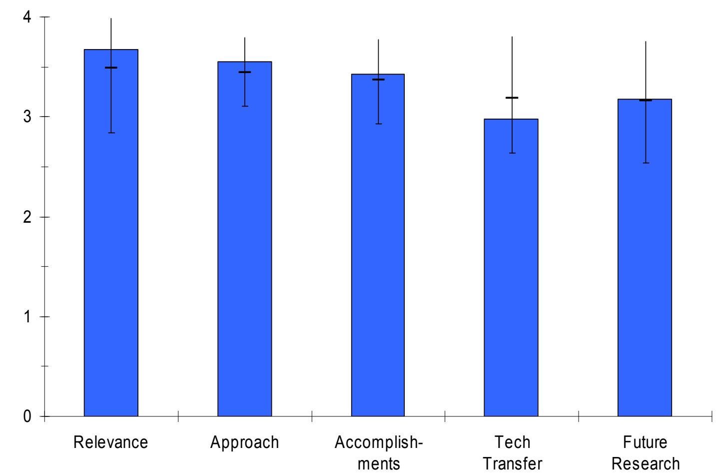
Specific recommendations and additions or deletions to the work scope

- Add more analysis of the vehicle performance.
- More information on the deployment of the new generation fuel cell vehicles. How are they going to analyze the differences between the first and second generation?
- Provide data on climate conditions.
- It would be interesting to see DCX get interested in some integrated fuel-CHP activity, rather like the home refueling projects done by other companies.
- Please provide data on the key parameters – to promote positive and beneficial features of FCV and hydrogen.
- In the future, this presentation should focus much more on strictly technical/engineering outcomes from the testing.
- The approach based on sending all data to NREL does not seem to work; among others, it does not allow to discriminate between different teams' progress – their strengths and weaknesses; test summaries, lessons learned and conclusions should be delivered by individual teams, not combined and "averaged" by NREL.
- There seems to be a need to resolve codes and standards issues before building more hydrogen filling stations.
- Per-dollar value of this and other technology validation projects should be reviewed by DOE.

Project # TV-02: Hydrogen Fuel Cell Vehicle and Infrastructure Demonstration Program Review
Greg Frenette; Ford

Brief Summary of Project

Overall Project Score: 3.4 (4 Reviews Received)



To date in this project, Ford has placed 18 Gen I hydrogen fueled vehicles in fleet user service in three varied climatic regions to demonstrate the efficiency, reliability and durability of the fuel cell power concept, and to validate the concepts through the collection of real world data. To date, these vehicles have accumulated 274,000 miles. In parallel, hydrogen fueling stations have been sited (City of Taylor, MI, Jamestown, FL and Sacramento, CA Airport) to establish an initial hydrogen infrastructure, demonstrate alternative hydrogen production concepts, and evaluate production technologies for cost effectiveness. Emerging technologies in vehicle and hydrogen infrastructure are being validated in separate, advanced engineering vehicles (Gen II) and fuel cell system designs that demonstrate improved functionality, range, durability, economy, weight and cost.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.7** for its relevance to DOE objectives.

- Project is important effort to demonstrate the feasibility of fuel cell vehicles and hydrogen infrastructure.
- Project is well aligned to DOE goals. Gathering data on a number of vehicles in several locations and also collecting fleet experiences is important to understand the true status of the technology in real-world applications.
- A status of cost reduction progress would improve relevance.
- Acquiring "real-world" operational data and experience is vital to making appropriate adjustments to the hydrogen R&D project mix and specific projects.
- This project is generating significant operational data.

Question 2: Approach to performing the research and development

This project was rated **3.6** on its approach.

- Good distribution of fueling sites with varying weather conditions.
- Good plan to demonstrate the technology and address specific issues through controlled tests and developmental prototypes.
- Crash safety studies should be included.
- Changing of an infrastructure objective was a good adjustment.
- Design of a multi-faceted gen 2 has resulted in a sound approach to addressing specific challenges that have been identified.
- Results and data from initial operations are being incorporated into next generation designs.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.4** based on accomplishments.

- Not meeting miles driven or hour targets, but getting better.
- Good fuel cell performance.
- Fueling infrastructure issues are significant, specifically high cost and low usage.
- Excellent progress made so far. Vehicles being operated and fueled in all planned locations.
- Good list of lessons learned for infrastructure. This is important to share with industry to avoid making similar mistakes with future installations.
- Gen 2 vehicles progressing well: could go a long way to gain consumer acceptance especially by reducing the intrusion into cargo space.
- Suppliers of components should be involved with a high volume assumption to drive costs down.
- Reported on accumulation of vehicle miles versus targets.
- 8 of 18 gen 1 vehicles projected to achieve mileage and hours targets.
- Outstanding discussion of gen 2 prototype program. Excellent progress in past year on development of gen 2 vehicles.
- Outstanding attention to safety issues and concerns.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- Data are being provided.
- Good partnership arrangement.
- Working with first responders to ensure adequate training and awareness.
- Good collaboration and coordination between team members.
- Collaborations outside the project team not apparent from presentation.
- It appears that more university and DOE lab assistance should be solicited.
- No discussion of outreach, training activities in the presentation.
- Communications on the project with other than the partners seems to be limited, based on the information provided.
- In response to a question, declined to provide any details to support conclusions/lessons learned.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.2** for proposed future work.

- Continuing current effort with some improvements to vehicles and stations.
- Hybrid configuration could be interesting compromise to hydrogen storage challenges.
- Future plans include continuous improvement to vehicle design, specifically with hydrogen storage.
- Consumer research should be included.
- Discussion of future research was limited and general.

Strengths and weaknesses

Strengths
- Experienced partners.
- Project partners are continually improving vehicle design by addressing technical issues with sound R&D.
- Solid project plan – multiple vehicles in service in different climates to demonstrate technical progress.
- Showing cost reductions in new designs
- Great engineering and fabrication are evident. Results of testing are excellent.
- Getting significant miles and hours on vehicles.
- Gen 2 vehicles show promise of significant improvements.
- Attention to safety.

Weaknesses
- Results from customer feedback on performance and experience should be included in presentation.

- Needs more collaboration with labs, universities, and suppliers to move toward real world, affordable products.
- Little evidence that there are education and outreach activities as important elements of this project.
- It is not clear that benefits per dollar spent are maximized, due to the dispersion of hydrogen infrastructure sites built specifically for the project and so few vehicles.

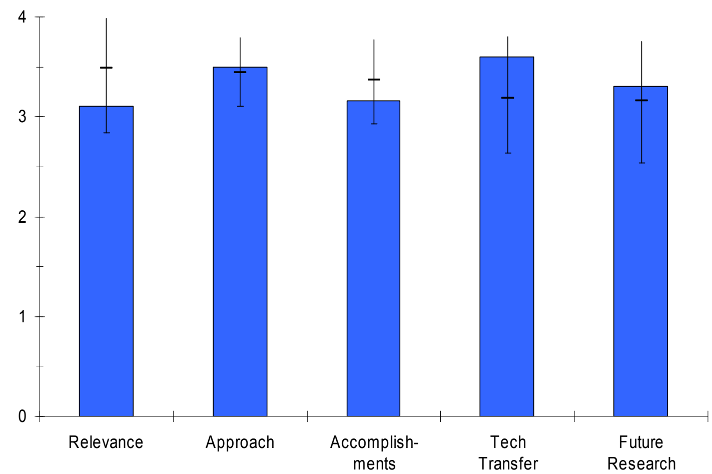
Specific recommendations and additions or deletions to the work scope

- Increase miles driven and the number of vehicles available so that stations can be more fully utilized and more information on potential improvements generated.
- If possible, some baseline comparisons with conventional technology in similar service would help show the progress toward commercialization.
- Please search for ways to make more of the data and information generated by the project publicly available. More should be shared in exchange for public (Federal) funding of $44 million.

Project # TV-03: Controlled Hydrogen Fleet and Infrastructure Demonstration and Validation Project
Dan Casey; Chevron

Brief Summary of Project

Overall Project Score: 3.3 (5 Reviews Received)



Chevron, Hyundai-Kia Motor Co. and UTC Power are conducting a five-year demonstration and validation project designed to showcase how fuel cell vehicles (FCVs) and hydrogen infrastructure can be designed to work together to fuel vehicles of the future. The primary goal of this project is to demonstrate up to six hydrogen energy stations (primarily in Southern California, with one site elsewhere to test cold climate conditions) and up to 32 FCVs as well as inform key audiences about hydrogen as a potential vehicle fuel. Both cold- and hot-weather testing was conducted in the past year. In addition, important safety and legal codes and standards for hydrogen refueling technologies will be developed in conjunction with the federal government and other authorities. Hyundai will provide a fleet of up to 32 vehicles, powered by UTC fuel cells. Hydrogen at the refueling stations will be generated using different types of natural gas reformer technologies and electrolysis. Other collaborators include Southern California Edison, Hyundai KIA America Technical Center, Inc., Alameda Contra Costa Transit and Tank Automotive Research, Development and Engineering Center, who will serve as vehicle fleet operators and site hosts for hydrogen fueling and power generation stations.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.1** for its relevance to DOE objectives.

- Excellent description of objectives. Very clearly stated.
- Good demonstration program but there are no R&D objectives here.
- Necessary activities to move forward with fuel cell testing coupled with fuel infrastructure development.
- Excellent match with DOE targets and President's objectives.
- This is one of several highly visible and very expensive projects that are not very likely to have a major impact on overcoming the greatest challenge of the Hydrogen Fuel Initiative.

Question 2: Approach to performing the research and development

This project was rated **3.5** on its approach.

- Their approach is right on target with what DOE wants.
- Impressive number of vehicle. PI needs to explain if this is Gen 1 or Gen 2 vehicles like the other automotive OEMs. PI needs to clarify if these vehicles are freezable or not.
- Chevron is doing what needs to be done. The GRI program is interesting, with an option to make either hydrogen or electricity. Excellent emphasis on training and education.
- Excellent combination of FC manufacturer, vehicle supplier, and energy provider as well as sites and users.
- Keep hydrogen capacity low to match with the anticipated FCV usage and hydrogen (keeps cost low!).
- Virtual absence of technical content in the presentation makes the approach taken difficult to assess.
- A list of milestones does not constitute an approach.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.2** based on accomplishments.

- Good training with first responders.
- All station progress clearly explained
- GTI POGT (Gas Technology Institute Partial Oxidation Gas Turbine)
- Hot and cold weather results clearly explained. Data collection explained. Lessons learned for storage inventory calculation.
- Looks like infrastructure lags behind vehicle deployment quite a bit. It would be unreasonable to expect many miles until next year's Merit review.
- Good progress in getting the fueling stations operational. Several different locations with different climates are involved. Data collection is well done, focused and intelligent.
- Good progress towards number of vehicles and refueling stations.
- 350 bar readiness is good.
- No mention about range and benefits/challenges of 700 bar FCV.
- Please provide data on your experience for customer benefit (range, miles/kg, emissions, etc)
- For the reason of very scarce technical information, progress evaluation is extremely difficult.
- As in the case of other technology validation mega-projects the value-for-money aspect of the Chevron project continues to be unclear.
- Reporting data to NREL cannot be used as a measure of progress and accomplishments; that data should have been included in the presentation.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.6** for technology transfer and collaboration.

- Not too many partners to drive the cars around. PI should have a slightly larger group for diverse driving patterns.
- Quality project team.
- Very good combination of stakeholders and productive outreach activity.
- Numerous, strong partners from various sectors.
- Coordination and division of effort have not been sufficiently addressed.
- Based on this presentation alone, UTC's role in the project is unclear (except for providing a winter-test venue).

Question 5: Approach to and relevance of proposed future research

This project was rated **3.3** for proposed future work.

- 32 cars in 2007.
- Pretty straight forward here what needs to be done in the next few years.
- More cars, more miles, more data – all the right direction. The GRI effort brings on-site hydrogen to the mix.
- Good plan.
- Learn about different climates.
- Validate POGT benefits.
- Proposed future research merely represents continuation of the testing; there seems to be no impact of previous research on future plans.
- Once again, the project suffers here from the lack of technical information that should have served as a base for future research.

Strengths and weaknesses

Strengths
- Real world data being collected

- 6 on site generators being tested.
- Cars on road in all climatic conditions.
- Excellent team; solid planning.
- Good combination of climates and civilian vs. military sites.
- 20 vehicle deployment is an excellent progress and commitment from the team.
- In spite of the absence of specific technical information from the testing, one might assume that significant number of test data has been generated in this testing and delivered to NREL.

Weaknesses
- None identified
- A little bit behind the other automotive OEMs.
- No projected performance on POGT or lab data for hydrogen.
- What is the impact on emissions due to POGT?
- Very little technical information has been made available to the community.
- Like in other technology validation projects in this group, the benefit to the manufacturers of the key fuel cell components is questionable at best.
- Approach based on sending all the technical information to NREL does not seem to have worked very well and made project evaluation virtually impossible.

Specific recommendations and additions or deletions to the work scope

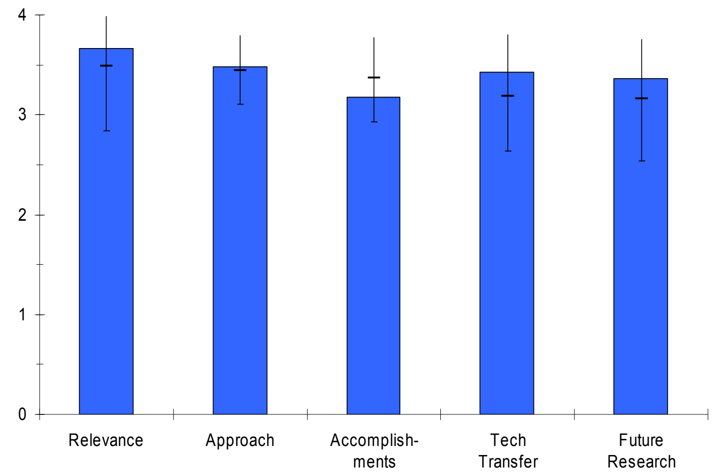
- Analysis on the cost of hydrogen delivered.
- Automotive partner needs to give it to a little more diverse group of customers.
- Teams in charge of this and other technology validation mega-projects should be required to deliver real technical presentations from their work; at present, the use of NREL as an intermediary produces an average over the outcomes of all teams, with relatively little information that could be truly useful for advancing the hydrogen technology.
- Huge investments of DOE funds in technology validation projects led by Chevron, DaimlerChrysler, Ford and GM ought to be re-assessed.

Project # TV-04: Hydrogen Vehicle and Infrastructure Demonstration and Validation
Roz Sell; General Motors

Brief Summary of Project

General Motors and energy partner Shell Hydrogen are deploying a system of hydrogen fuel cell vehicles integrated with a hydrogen refueling infrastructure to operate under real world conditions to: 1) Demonstrate progressive generations of fuel cell system technology; 2) Demonstrate multiple approaches to hydrogen generation and delivery for vehicle refueling; and collect and report operating data. Eight gen 1 vehicles have been deployed in Washington, D.C. and southern California. This project will demonstrate two generations of fuel cell technology deploying forty fuel cell vehicles (8 gen 1 and 32 gen 2) fueled with hydrogen from stations in five locations.

Overall Project Score: 3.4 (5 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.7** for its relevance to DOE objectives.

- Vehicle OEM demo partnerships with fuel suppliers are square in the middle of the DOE Technical Validation Scope.
- Strong team with focus on meeting Hydrogen Initiative goals through well-designed vehicle and infrastructure demonstration project
- Project is in line with DOE objectives – results of real world experience is important to assess technology readiness.
- The PI addressed everything in an outstanding way.
- Acquiring "real world" operational data and experience is vital to making appropriate adjustments to the hydrogen R&D mix and specific projects.

Question 2: Approach to performing the research and development

This project was rated **3.5** on its approach.

- Lack of progress in deploying hardware belies an apparent weakness in approach.
- The Shell early accomplishment in getting the Benning Road station up and running was apparently out of sync with vehicle deployment.
- Incorporation of hydrogen into existing fueling sites is great way to introduce the public to the idea of hydrogen as an alternative fuel.
- Bi-coastal approach hits areas with diverse climate and large populations, in addition to strong political interest.
- Public access fueling stations are a good approach – can lead to other hydrogen vehicle partnerships that leverage limited funding and increase station use.
- Documenting C&S and permitting imperative to share success and difficulties. Can help future projects avoid the same issues.
- Suppliers should be heavily involved. A cost study trend should be developed to track progress toward reality.
- Approach results in anticipated benefits being concentrated in the latter half of the project period. Will increase the vehicles by a factor of 4, and expand fueling sites from 1 to 3.
- Placing stations at retail sites is a plus for the project.
- Project elements of outreach to students, training of first responders and showcase events are outstanding.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.2** based on accomplishments.

- Despite high profile announcements and photo ops, real deployment of fuel cell vehicles has not occurred.
- 8 vehicles (not much used) and 1 refueler are not in keeping with initial expectations.
- Other similar projects have resulted in dozens of real, roadworthy vehicles each in service with hundreds of non-professional driver experiences.
- Making progress and expanding into new cities as planned.
- Recognize permitting issues as the longest lead item.
- Great progress made in the last year with putting vehicles in service and fueling stations on-line.
- Would like to see some general descriptions of how the vehicles are being used by each site.
- New vehicle is outstanding.
- Based on presentation information, there is no way to assess vehicle and re-fueling infrastructure performance.
- Even minimal information on vehicle miles and hours was not mentioned, and not offered in response to a question.
- Detailed information was provided on some topics, e.g., education initiatives, but not with respect to issues.
- Related to major commercialization barriers.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.4** for technology transfer and collaboration.

- The Shell refueler at Benning Road has been a very good opportunity to show policy makers and the general public that hydrogen can be handled safely and be available conveniently.
- The addition of the State of Virginia Department of Environmental Quality and USPS as project partners has offered high profile additional opportunities to deploy vehicles.
- Well integrated partners, with complete, or nearly complete, set of skills at high level.
- Good set of recommendations/observations related to key challenges and suggested approaches for solution.
- Project team working well with other groups to transfer knowledge: training program with first responders excellent.
- More involvement of DOE labs and universities should be included.
- Outstanding number and diversity in vehicle operator partners. In gen 2, will be getting data from a variety of drivers.
- Good discussion of data design and transfer system.
- Outreach and education are important in this project.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.4** for proposed future work.

- The proposed 100 new vehicles is a promising new beginning after a slow start.
- The use of non-professional drivers in this new phase will be a welcome new opportunity.
- Expansion into other large markets fits strategy well.
- Future work planned will add data on many more vehicles in service, which will be important to help meet DOE tech targets.
- Data collection from customers and other participants are a good addition to the overall project.
- Sales and marketing research should be part of vehicle research.
- The major benefits from this project seem to lie ahead, in gen 2.

Strengths and weaknesses

Strengths
- The Shell Hydrogen partner seems reliable
- The addition of the USPS component is a good fleet option apparently missing from the initial four FreedomCAR projects.
- The photo ops for this project have been exceptionally well advertised; a benefit to all the FreedomCAR projects.
- Experienced and committed team members.
- Larger numbers of vehicles will provide a good baseline on the current state of the technology.
- Public station access creates opportunity for collaboration with other projects and helps build public awareness for hydrogen and fuel cell technology.
- Great engineering and fabrication are evident. Results of testing are excellent.
- Outreach, training, and education.
- Gen 2 vehicles show promise of significant improvement.

Weaknesses
- GM's lack of enthusiasm for vehicle deployments.
- Need to begin transfer of fueling and some maintenance to customers to gain real acceptance.
- None.
- Relatively little operational experience to date, with one re-fueling site and 8 vehicles.
- Reluctance to provide even basic specific results and data.
- It is not clear that benefits per dollar spent are maximized, due to the dispersion of hydrogen infrastructure sites and so few vehicles.

Specific recommendations and additions or deletions to the work scope

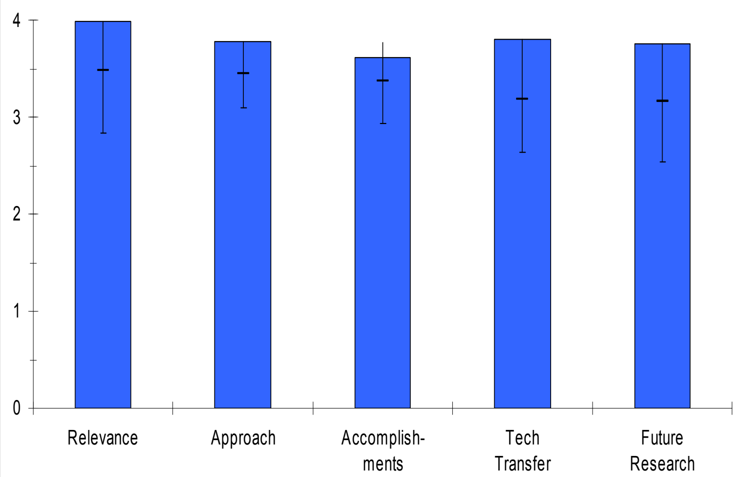
- Need to ensure that C&S efforts are fully integrated into the other Program activities in this area.
- Please search for ways to make more of the data and information generated by the project publicly available. More should be shared in exchange for public (Federal) funding of $44 million.

Project # TV-05: Controlled Hydrogen Fleet and Infrastructure Analysis
Keith Wipke; NREL

Brief Summary of Project

Under this multi-year validation project the National Renewable Energy Laboratory is assisting DOE in demonstrating use of fuel cell vehicles and H2 infrastructure under real-world conditions, using multiple sites, varying climates, and a variety of sources for hydrogen, including renewables. The objectives of this project include: 1) Validation of hydrogen fuel cell vehicles and infrastructure in parallel; 2) Identification of current status of technology and its evolution; 3) Re-focusing hydrogen research and development; and 4) Supporting the technology readiness milestone in 2015. This project takes data from all the controlled hydrogen vehicle and infrastructure fleet tests, analyzes it, and prepares reports.

Overall Project Score: 3.8 (7 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **4.0** for its relevance to DOE objectives.

- This project is exactly what DOE EERE needs to maintain the proprietary data.
- Excellent work to gather all TV [Technology Validation] information
- We finally can look objectively at the claims being made by GM, Ford, DC, and Hyundai.
- Critical effort to collect, organize, and distribute the fuel cell vehicle fleet data. Absolutely necessary to do this and do it very well because so many resources are being spent to do these demonstrations.
- Analysis of FCV fleets and utilization of hydrogen.
- Infrastructure is very important. The project address that well.
- Objectives are well defined and measurable.
- This oversight project is essential to assessing the status of hydrogen vehicle progress.
- This is the conduit to some of HFCIT's most important projects. It is very relevant.

Question 2: Approach to performing the research and development

This project was rated **3.8** on its approach.

- This project approach was designed in close coordination with DOE staff and is being conducted in a professional manner.
- Secure and analyze the data. HSDC (Hydrogen Secure Data Center). 114,000 individual trips analyzed.
- Interact with companies.
- Would like to see more public disclosure as soon as available.
- Excellent.
- An impressive activity by NREL, doing exactly what is needed. Intelligent plan. Proprietary concerns managed correctly.
- Good strategy for data collection and analysis.
- Need to identify key parameters to showcase the benefits of FCV and hydrogen (miles/kg, impact of operating conditions, maintenance, emissions, etc).

- Refueling time, amount, capacity factors, and availability factor should be analyzed for greater value of the data.
- The data presentation is comprehensive and thorough, considering the field experience in the program.
- Many database systems are used by industry to manage larger and more complex databases. It is not obvious that a custom database was necessary. It may have been more cost effective to use a commercial database rather than developing a DOE proprietary database for this single task.
- Putting the data on a website is an excellent improvement.
- “Mean Time between Failure” and “Mean Time between Repair and Availability” data would be good to add to the data set.
- “Fueling Station Fuel Delivery Capacity Factor” (capacity served as a percentage of available capacity) would be good to add to the data set.
- Some indication of stack life or stack changes would be good to add to the data set.
- This task is difficult. NREL uses a good approach, using the secure data center.
- NREL did not mention one of the key steps of their approach – gaining the trust of the four project teams. Good job!
- The series of publications is a good component.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.6** based on accomplishments.

- Fleet analysis Toolkit FAT is used.
- All methods are documented in quarterly reports. These have been delivered on time and have been presented at key conferences. 30 composite data have been published.
- Developed a more responsive website for easier access to users. This was in response to the previous annual program review feedback.
- They have determined the fuel cell stack hours accumulated through December 2006. Extrapolation was used to determine fuel cell stack degradation. They can determine the DOE target of 1000 hours degradation of 10%.
- Their safety reports provide some documentation of safety incidents.
- Infrastructure maintenance is important in identifying future maintenance requirements.
- Excellent.
- Excellent.
- NREL has done a great job during the first phase, and has built a quality team for continuing forward.
- Too many details, little substance, please focus on key results.
- On-road data is most important for customer acceptance.
- Please use graphics that are more legible.
- Progress is consistent with project progress and up to date – this is a strength.
- I think we're seeing good progress now. It was difficult for this project earlier before much data had been transferred, and there appeared to be some skepticism as to if they would obtain sufficient data.
- While there is certainly much sensitive data, it is unclear why the PI does not differentiate between data that is sensitive and cannot be reported and data which simply hasn't been analyzed. I sensed a hesitation to differentiate between the two. Reviewers can still get a feeling that the project is headed in the right direction if we are told that the analysis has been performed, but the result has not been cleared (or even won't be cleared).

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.8** for technology transfer and collaboration.

- They collect data from industry successfully and disseminate data via website very successfully.
- They compute a range from several sources based on their input.
- They can put the pieces together and determine a range histogram per company.
- Vehicle range factors analyzed include on road, window sticker and dyno (dynamometer) range.
- Great job of cooperation with teams and publishing results.
- Need to collaborate more with universities.

- Excellent cooperation with industrial, governmental and other (public) stakeholders. Excellent record of getting data distributed.
- Good interactions with stakeholders.
- FC [fuel cell] and refueling station should be separately addressed and analyzed.
- Data dissemination using a website is an excellent improvement.
- The listed collaborations with other projects are excellent.
- The reports and website are a real plus.
- Interfacing is by definition controlled.
- Safety Panel interaction is very important.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.8** for proposed future work.

- Stack degradation data will improve as more hours are reported per stack.
- Radio histogram of refueling.
- Feedback for future R&D.
- Encourage expansion to include MTBF [mean team between failures] and FMEA [failure mode and effects analysis] information as more data is collected.
- Excellent.
- One hopes for the same quality as NREL gave for gen 1 plus even more.
- Fuel cell degradation under hybrid vs. non-hybrid (more demanding conditions) should be analyzed. This will help R&D to better focus on the duty cycles.
- Compare with others in non-DOE environment if possible.
- Next phase plans are appropriate and timely.
- Exactly what it needs to be.
- Compilation of lessons learned, especially in the safety area would be welcomed.

Strengths and weaknesses

Strengths
- Provides DOE with a means to analyze collect data and analyze it in a methodic way. Excellent dissemination of data.
- Great analytical capability great data handling capability.
- Data collection algorithms and comprehensive analysis.
- Good summary of progress made, overall status.
- Web-access of reports is great progress.
- Breadth of data.
- Lessons learned.
- Customer data (time to refuel).
- A very tough job, done well.

Weaknesses
- None
- Inhibited by need for confidentiality.
- Need to filter out the "noise" and "bias" of the data input. A question of veracity.
- Please minimize the introductory slides that do not contribute to the project message (e.g. slides no. 11, 12, 13, 14, 15, 27-28, etc).
- No comparison with other international projects.
- Some programs are not tracked (APS for one).
- See second bullet under technical accomplishments. [While there is certainly much sensitive data, it is unclear why the PI does not differentiate between data that is sensitive and cannot be reported and data which simply hasn't been analyzed. I sensed a hesitation to differentiate between the two. Reviewers can still get a feeling that

the project is headed in the right direction if we are told that the analysis has been performed, but the result have not been cleared (or even won't be cleared).]

Specific recommendations and additions or deletions to the work scope

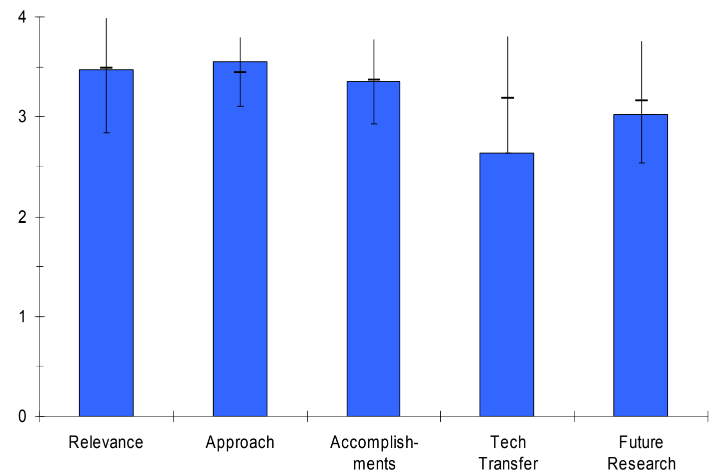
- 40 slides in this venue are a bit much to absorb.
- Suggest policy options to assist car manufacturers and energy providers to commercialize vehicles and establish critical infrastructure.
- Lessons learned would be helpful as a published report.
- Other countries (i.e. Asia and Europe) have somewhat similar fleet operations underway. It would be interesting to build a global record of fuel cell vehicle demonstration results. At least, NREL might add some web links so those reports are easy to find.
- Focus on lessons learned – identify positive attributes for good value – highlight them.
- Capacity factor at each site is important for cost reduction.
- Benchmark against European and Japanese initiatives
- Try to include more projects, even those not in the DOE program.
- Compilation of lessons learned.

Project # TV-06: Validation of an Integrated Hydrogen Energy Station
Dan Tyndall; Air Products

Brief Summary of Project

Air Products and Chemicals, Inc. is conducting a project to demonstrate the technical and economic viability of a hydrogen energy station using a high-temperature fuel cell to produce hydrogen and electricity. A total system design and engineering development effort has been completed with the goal to economically recover hydrogen from the anode of a high temperature fuel cell. Design and construction of the energy station is in progress. The project will conclude in a year-long demonstration of the system at a suitable site. Safety is the top priority in the system design and operation.

Overall Project Score: 3.3 (6 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

- Excellent concept for pursuing energy-generating infrastructure.
- Reduced hydrogen cost and improved efficiency extremely beneficial.
- This project is advancing capability on the supply side.
- Production of heat, power and fuel from waste streams could provide environmental benefits with respect to both the elimination of waste and production of useful energy products.
- Project addresses the lack of hydrogen infrastructure for hydrogen which fits into DOE objectives.
- Need to indicate how much of these sources are available in a practical manner. (Is digester gas a potential to supply 1% or 10% or 50% of U. S. needs?) Without this info the relevance is very hard to access.
- Demonstrating the viability of using a variety of biomass feedstock materials to produce hydrogen at commercial prices.

Question 2: Approach to performing the research and development

This project was rated **3.6** on its approach.

- Thorough project design.
- Appropriate correlation with natural gas pricing – cost reduction should be focused on improvement of conventional storage, clean up, compression, balance of plant, and dispensing systems.
- Further explanation of cost saving opportunities is needed, if any, of new PSA technology/design.
- Project has many parts to it, and appears organized to adequately handle all parts.
- Right-sized for the streams of interest.
- Flexibility of the system allows it to be used with a variety of feedstocks that are not necessarily available in huge quantities.
- Good approach for station capable of producing hydrogen fuel and providing electric power.
- Allowing for multiple feedstocks makes the system more flexible for use at varying geographic locations.
- Excellent plan and execution to date.
- In his presentation, and response to questions, Mr. Tyndall clarified the importance and challenge of: (1) integrating equipment included in the overall system design; and (2) design of the sub-system for hydrogen purification.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.4** based on accomplishments.

- Excellent design and planning; timeline for completion looks good.
- Permitting is critical, further discussion of progress to completion needed to verify timeline.
- Project schedule moving a little slower than expected relative to state of project presented last year; e.g., Advanced PSA H_2 recovery was already done last year, so intervening time has only produced bid specs and some (very important) gas clean-up work.
- Progress would likely have been more advanced if DOE funding had been more available.
- Making good technical progress.
- Site selection for Phase 3 facility.
- Project appears to be on track.
- Excellent choice of sites: having a motivated partner will greatly improve chance of a successful demonstration.
- Early days yet, but looks very promising.
- Has taken quite a while for the project to hit its stride (only 20% of the budget so far). But preliminary work prior to final design and construction has been thorough, resulting in well-supported decisions which should set the stage for a successful demonstration.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.6** for technology transfer and collaboration.

- Partnership with FCE appears positive and ideal.
- Interfacing with potential users (OEMs) is unclear.
- With the several elements in the project and public demonstration, this is an excellent opportunity to build new working relationships and capability among important supplier and user groups.
- With the selection of the site for Phase 3, relevant partners are being identified.
- Technology transfer not apparent from presentation.
- Need more industry, universities, and DOE labs involved to address design refinement opportunities and reduce cost.
- Based on the presentation, there is no evidence of collaboration or communication with organizations other than the project participants.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- On paper the numbers (e.g. efficiencies, production, power, etc.) are incredibly promising – real-world performance data are critical to project success.
- Data collection and real-time performance analysis plan is unclear.
- The group is identifying and solving issues as presented.
- This project is revealing work needed in gas clean-up.
- This project is revealing relative value to production of H_2 vs. electricity.
- Future design progress for the selected site will focus the work on this specific feedstream, and will allow APCI to optimize the process design and operation.
- Need to document the experiences and lessons learned, including user perspective.
- Need to work with user to include hydrogen vehicle fueling as part of project. System can't be fully demonstrated without testing that aspect along with power generation.
- Study total long term potential for significant percentage of H_2 and electricity for total country needs.
- Plans for completing Phase 3 and later phases follow logically from the planning, design work and studies accomplished during the earlier phases of the project.

Strengths and weaknesses

Strengths

- Excellent and needed project concept: energy + hydrogen + heat + bio-waste energy.
- Potential to fill real-world data needs for energy stations and bio-waste energy/hydrogen production.
- Waste-to-energy projects are very desirable at the community level. This project provides a renewable energy hydrogen production application while showing how technology can truly help solve the burdensome problems of waste disposal.
- Good progress on operation of PSA for dilute hydrogen feed.
- Multiple feedstocks make the system more flexible.
- Very promising for very low cost H_2 and electricity production.
- Builds on technology for power production that is becoming more widely used, and for which there is a growing experience base.

Weaknesses

- High project complexity including added new technologies with unclear cost advantages (e.g. new PSA).
- Greatest value to come from installed, working station generating real-world data – permitting and other external factors will greatly influence timeline (real-world operation less than one-half of overall timeline).
- This project seems to be going a little slower than I expected. Perhaps I'm just too anxious to see this integrated project get going.
- Need to transfer lessons learned and document process of gaining permits to build station. This will be important for the industry and others interested in implementing the technology in the future.
- Acronyms are excessive. (I missed some info I'm sure.) Concerned if all this effort has potential for a significant amount of H_2 and electricity on a total country percentage effect basis.
- Evidently the project budget will be increasing, in order to allow completion of work currently planned for Phase 3 and beyond.

Specific recommendations and additions or deletions to the work scope

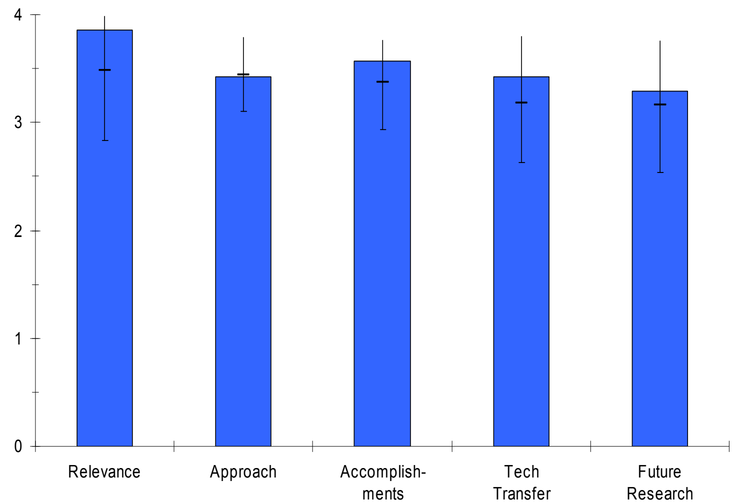
- Extended operational term with comprehensive data gathering covering efficiency, well-to-wheel emissions and energy use.
- Lessons learned and barrier identification for future commercial infrastructure.
- Based on my experience with trying to develop similar projects in Sacramento, I have difficulty accepting the economics as presented. Maybe this project needs to disclose actual project costs for components as well as projected future costs.
- Work with project partners (or add partners) to fully test system capabilities by adding hydrogen vehicle fueling demonstration.
- Calculate how much total energy (%) the USA could get long term!
- A statement was made indicating there is some interest in adding a hydrogen fueling station to the project. If that happens, it is recommended that DOE not participate in funding such an addition to the scope, since DOE is already supporting a number of demonstration hydrogen stations.

Project # TV-07: California Hydrogen Infrastructure Project
Ed Heydorn; Air Products

Brief Summary of Project

This project is focused on demonstrating a cost-effective hydrogen infrastructure model in California for possible nationwide implementation. It includes the design, construction and operation of seven hydrogen fueling stations; collection and reporting of operational data; documentation of permitting requirements and experiences; and validation of expected performance, cost, reliability, maintenance, and environmental impacts. In this project Air Products is also deploying a novel hydrogen compressor they have designed with capital costs potentially 50-75% less than conventional systems. This project will also implement a variety of additional new technologies with the objective of lowering the cost of delivered hydrogen.

Overall Project Score: 3.5 (7 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.9** for its relevance to DOE objectives.

- Most relevant aspects include fuel station footprint reduction and infrastructure capital cost reduction.
- Learning and value gained by increasing vehicle usage and infrastructure learning through the creation of a working "network".
- Additional value generated through innovative, new technology developments – greatest DOE value gained if learning is shared.
- 7 fueling stations are targeted. Results are being compared to NREL's data. This project helps DOE determine a transition pathway for establishing hydrogen fueling stations from several different sources.
- Very relevant to the DOE objectives for H_2 cost and delivery.
- Understanding the cost associated with development of a hydrogen delivery infrastructure is important to the future of hydrogen vehicles.
- Validation of the technology is on the critical path to establishing a hydrogen energy structure in the U.S.
- Direct application to immediate use for H_2 fleet. Excellent transient filling stations.
- The DOE emphasis on testing and evaluation of hydrogen vehicles requires the deployment of a hydrogen infrastructure. This project is a part of this emphasis.
- Hydrogen refueling stations are vital to the president's initiative – this is a very important contribution towards that goal.

Question 2: Approach to performing the research and development

This project was rated **3.4** on its approach.

- Excellent work with OEMs in coordinating fuel demand vs. location vs. timing and fueling requirements
- Reliance on mobile and temporary stations may limit extrapolation and learning for future commercial infrastructure deployment, cost and footprint reduction as well as reducing the "retail"-feel for near-term customers – future work and presentations should clearly show linkage of mobile application learnings to future commercial situation
- Work with OEM's and station operators.

- Design, permits, and installation are detailed.
- Specific status relative to technical/cost barriers was not sufficiently addressed.
- Unclear if sufficient detailed information will be provided to DOE to help guide R&D.
- Project should benefit Program by involving OEMs not currently involved in the learning demos.
- Criteria for success, cost targets, milestones, etc., are unclear.
- The approach is well organized and addresses many of the critical features to making the hydrogen station a commercial enterprise.
- The collection of data and feedback for the station operations is an important aspect for the next generation of hydrogen delivery systems.
- Very focused effort on new compressor may be diluting effort by inclusion due to development required.
- Main emphasis is validation of performance. Most of this project seems a conventional business activity, selling and installing commercial hardware; in this role Air Products serves more like a vendor.
- Working with all stakeholders including OEMs and energy companies.
- Is a great approach – from planning through execution stages.
- Selection of low-cost alternate designs to reduce the cost of hydrogen.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.6** based on accomplishments.

- Progress to date is impressive, particularly for the new UCI station with 700 bar fueling and a more "retail"-like setup – further developments of this kind should be pursued.
- Progress on novel compressor appears promising – reduced capital costs clear, however, the operating costs and electricity usage (energy use) need to be better explained.
- UCI has 300 fills and have met all performance targets.
- This is a public station. Opened in February 2007.
- Torrance station based on Air Products pipeline as a source of hydrogen. Completion should be ready by the end of 2007.
- Hydrogen Fuelers (HF-150) mobile fuelers. This is being held in Long Beach, CA. The station should be online in the next 30-60 days.
- New delivery concept – trailer delivered with gaseous delivery on demand. Testing is completed. Hydrogen Base Unit (HBU) hydrogen fueler without wheels. Discussing the HBU with station operators to help in the transition. Novel compressor system is being integrated with these stations.
- Good technical progress since last year.
- Progress in site selection has been slow.
- Some unique delivery concepts and a compressor are included that should benefit the Program and help support near-term activities by OEMs.
- Program progressing well. Start up of fueling stations at UCI is important milestone.
- The presentation did not discuss the database that was developed but rather reported the event: reads somewhat like a press release not a technical program sponsored by the DOE.
- Novel compressor is interesting but is an adaptation of older technology. This should be identified by Air Products.
- Good implementation progress. Good scale up to 700 bar.
- Progress is evident in the UCI filling station. The pipeline project (Torrance) will be interesting to monitor. The portable tube trailers must be thought of as just a stop-gap activity.
- UCI stations with 350 and 700 bar capability show excellent progress.
- Mobile fuelers with liquid and gaseous hydrogen is a highly innovative low-cost option.
- Single stage [compression from] 100 psi to14000 psi without external cooling has a potential of cost reduction.
- Good use of APCI's (Air Products and Chemicals, Inc) experience in high pressure H_2 in other areas.
- Considering the funding used so far, excellent progress has been made in all seven stations.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.4** for technology transfer and collaboration.

- Good interfacing with OEM project partners.
- Unclear interface with other DOE TechVal (TV) programs – project managers should show linkage with TV programs and, if not already, develop appropriate systems to increase the overall network, vehicle usage, and learning generation.
- Well-to-wheels analysis to be conducted by UCI is a critical program feature.
- Many good collaborations are included in this project.
- Works closely with OEMs and fueling station operators especially Orange County and Los Angeles County in and around their pipelines.
- Very good collaboration with state and local entities in California.
- Program collaboration is within the program. I did not see much on outreach efforts.
- Will Air Products make station performance data available to all of industry or is this company private?
- The pipeline approach is unique to Air Products and should provide valuable information that could move the hydrogen infrastructure forward.
- Appears to have excellent communications with automobile people as well as station operators.
- AP has sought siting input from vehicle manufacturers. It would have been better to contact local agencies for a parallel input.
- Involving UC Irvine as outreach and study partner is an excellent idea.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.3** for proposed future work.

- Novel compression shows excellent capital cost reduction. Operating costs and energy usage need better explanation.
- Learnings from mobile fueler and new delivery concept deployments need to show clearer application to impacting future fully commercial infrastructure design.
- Novel compressor development – complete operating program (what about cost?).
- Their slide of future work was comprehensive and provided a good summary for each of the technologies.
- Report the costs and technical challenges of establishing a fueling station that uses an existing pipeline as the source.
- Future work will contribute to the Program with multiple operating H_2 delivery concepts and a novel compressor.
- More emphasis should be placed on addressing specific barriers and targets.
- Program planning is well organized and addresses the high points of the objectives.
- A commitment to share more data with the public would be a beneficial addition.
- Expanded installations excellent. Suggest new 14,000 psi compressor development effort be separated into its own project.
- Installation of hydrogen dispensing at other sites is an obvious follow-on, but was not mentioned.
- 700 bar vehicle support is important to increase the range. UCI station is ready for that.
- NDC (new delivery concept) and HBU (hydrogen based unit) testing is likely to provide a new low-cost option.

Strengths and weaknesses

Strengths
- Flexible and (relatively) short turnaround on infrastructure deployment concepts.
- Cost and footprint reducing technologies.
- 700 bar fueling for next generation vehicles.
- Well-to-wheels analysis of various deployment approaches.
- Integrates previously funded projects such as the novel compressor.
- Beneficial project as part of the initial H2 transition.
- Strong technical capabilities.
- Well organized approach by a strong company.
- Pipeline approach is very important to resolving delivery of hydrogen issues.

- Strong, workable equipment developed experience with installation. Experience with installation. Experience with a variety of fueling options.
- Working with all stakeholders and building on APCI's (Air Products and Chemicals, Inc).
- Technology strength is very important.

Weaknesses

- Heavy reliance on mobile and temporary station design may prohibit learning transfer to future commercial situation and may limit near-term development of a true FCV fueling network including a "retail"-feel for near/mid-term customers.
- None.
- Unclear if there will be sufficient dissemination of detailed results (such as costs) as input to the DOE technical targets to help guide future R&D.
- Program does not report like a DOE Technical Validation program. The same information was available to the press and the data exchange appears to be a press release. DOE programs should strive for a higher level of quality than a press release.
- Limited to distribution of gaseous and liquid hydrogen; no on-site generation options.
- Others have previously built and deployed compressed and liquid hydrogen portable hardware (fed by liquid hydrogen); so the N in the Air Products New Delivery Concept is not 'new". It takes considerable energy and diesel fuel to haul hydrogen around southern California, especially in tube trailers. There should have been a consideration of emissions resulting from the distribution of "clean" hydrogen.
- Perhaps beyond the scope – how to increase the capacity factor for the refueling stations.
- Identify transition strategy.

Specific recommendations and additions or deletions to the work scope

- Regular reporting of deployment lessons learned and critical barriers identification.
- Improvement of "retail"-likeness of future stations, customer friendliness.
- Cost of integrating the novel compressor.
- Detailed cost and lessons learned report on establishing the fueling station associated with pipeline. Also the potential opportunities should be documented including a detailed forecast of potential stations that could be converted between 2012 and 2015 if the demand exists.
- Adjust program to provide more technical exchange.
- Add on-site generation i.e. reformer and/or electrolysis options.
- California is making quite good progress in building hydrogen fueling stations i.e. the Hydrogen Highway. The DOE needs to be well integrated with this larger activity. Emphasis needs to be on standardization of systems and codes and standards so that costs can come down, and then on the building of a competitive commercial industry that builds the same station over and over again in many locations. One way this could happen is to set subsidies for these filling stations, and then lower those subsidies as the total number in place increases. This shot-gun approach, different technologies that include component development (that long, long promised AP hydrogen compressor), is not a route on the pathway towards a cost effective hydrogen infrastructure.

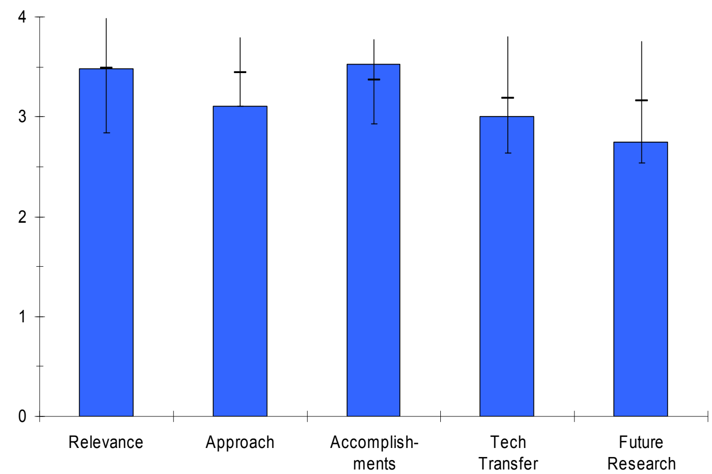
Project # TV-08: Cryogenic Capable Pressure Vessels for Vehicular Hydrogen Storage

Salvador Aceves; LLNL

Brief Summary of Project

The objective of this Lawrence Livermore National Laboratory (LLNL) project is to demonstrate long range (200 to 500 mile) hydrogen hybrid vehicle with an insulated pressure vessel. Insulated hydrogen pressure vessels have lower cost and safety advantages relative to compressed and liquefied hydrogen storage (e.g., no boil-off losses). The second generation insulated pressure vessels built by LLNL filled with liquid hydrogen can meet the 2007 volume and 2010 weight DOE targets (neglecting accessories). Future work will include development of improved insulated pressure vessels that can meet the DOE 2010 volume goal using liquid hydrogen.

Overall Project Score: 3.3 (4 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

- Uses science to crack existing paradigms with a good outcome!
- Strong relevance to DOE targets for storage volume and weight.
- Interesting strategy to increase vehicle range.
- Extremely relevant and very worthwhile.
- The project addresses DOE goals related to hydrogen storage aboard a vehicle.
- The work demonstrates the potential for significant improvement in range between re-fuelings for hydrogen vehicles.

Question 2: Approach to performing the research and development

This project was rated **3.1** on its approach.

- Uses the tremendous capabilities of the LLNL facilities to inexpensively explore with prototypical hardware the practicality of their theoretically based storage concept.
- Overall technical approach appears to be sound.
- It is still unclear if the system will be practical or cost-effective.
- Insufficient attention to cost/feasibility analyses.
- Not clear (even though better than 700 bar) that it can ever be affordable at long-term, high-volume. A road map of potential ways to get to affordability needs to be constructed.
- The scientific inquiry by LLNL, including use of phase diagrams, resulted in some potentially very important results. It supported well a decision to move into design, fabrication and demonstration of a cryogenic storage system.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.5** based on accomplishments.

- They have successfully accomplished what they set out to do.
- I rate the dollar/accomplishment very high for this project.

- Good technical progress is being accomplished on the system.
- Very good results and excellent technical progress. Low-cost, high-volume manufacturing technology needs to be added.
- Outstanding amount and variety of work accomplished with limited funds.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- Project scope and short schedule did not encourage multiple parties; quite acceptable for this project
- Collaboration to date appears to be limited and insufficient.
- There is potential future collaboration with OEMs.
- Need more production manufacturing knowledge input to design.
- Based on the presentation, there is no evidence of collaboration or communication with organizations other than the project participants.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.8** for proposed future work.

- Work identified with this successful start is leading to new deployments in the future. This will present vehicle integration challenges because the concept really breaks the existing design and use paradigms for vehicle fueling.
- Two important technical issues were identified for future work.
- There is no apparent effort to consider costs, weight, volume, etc., and make a realistic assessment of system viability.
- Lacking vision on moving to reality of mass production.
- Identified and discussed the limited work to be accomplished during the remainder of the present project.
- No specific information provided about potential future research or demonstration activity.

Strengths and weaknesses

Strengths
- Science-based breakthrough in really new capability for storage options available to consumers for "not always liquid or gas" vehicle fuels.
- Relatively fast and inexpensive project!
- Strong technical team.
- Excellent ideas with test hardware well built and tested.
- Significant work was accomplished for a relatively small public expenditure.
- Work accomplished ranges from scientific inquiry/analysis through practical application in a vehicle. Few projects have such a range of activity.

Weaknesses
- Relies on vacuum for much of its practical configuration.
- The need to describe this really interesting and useful concept to policy makers.
- May introduce a new and unanticipated dimension to vehicle safety.
- Insufficient attention has been provided to costs and/or realistic assessment of system viability.
- How to commercialize?
- System-wide (well-to-wheels) linkage is not established. Specifically: (1) no evidence that availability of liquid hydrogen re-fueling is considered; and (2) energy implications of liquefying hydrogen for use as an energy carrier.

Specific recommendations and additions or deletions to the work scope

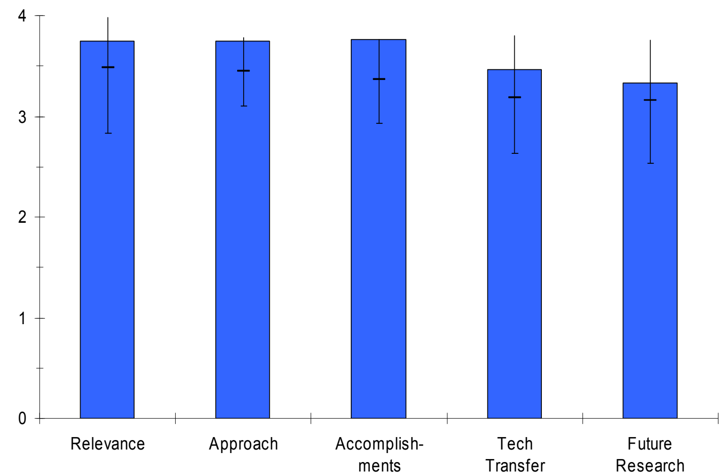
- Add (or initiate new project) to investigate possible new hydrogen release dynamics in a post failure mode. We know how gaseous hydrogen tanks behave in failure and we know how low pressure liquid behaves in tank failure. How would the spectrum of liquid/gaseous hydrogen behave? Describe the possible results in language appropriate for first responders.
- Project team should carefully examine potential costs and viability of system and include a go/no-go decision point before proceeding much further.
- Develop commercialization plan with suppliers.
- Before funding any further work on this system for storing hydrogen on board a vehicle, it is recommended that DOE perform analyses to address issues identified in the "Project Weaknesses" section above.

Project # TV-10: Technology Validation: Fuel Cell Bus Evaluations
Leslie Eudy; NREL

Brief Summary of Project

The overall objective of this project is to validate fuel cell and hydrogen technologies in transit applications by 1) showing progress of the technology toward commercialization, 2) providing "lessons learned" on implementing next generation fuel cell systems in transit operations, and 3) harmonizing data collection efforts with other fuel cell bus demonstrations worldwide (in coordination with the Federal Transit Administration (FTA) and other U.S. and international partners). To date, this project has collected operational, performance, and cost data on eight hydrogen fueled buses in real-world service at three transit agencies.

Overall Project Score: 3.7 (6 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.8** for its relevance to DOE objectives.

- Addresses fuel cell performance and durability data, infrastructure maintenance and training facilities.
- Validate fuel cell and hydrogen technologies in transit applications.
- Harmonizes data collection.
- Very relevant to the DOE objectives regarding cost, fuel cell durability, etc.
- Will help identify R&D needs.
- Good work and well-focused.
- This is needed for bus evaluations.
- The project objectives support DOE's objectives for gaining data and experience in fuel cells and infrastructure operations in a mass transit application. Key barriers are being addressed.
- Essential work gathering data on fuel cell bus operations. Critical that the data is collected and distributed by an "honest broker"; NREL fills this roll.
- Excellent summary of data generated from three bus projects in California.
- Buses provide the most important opportunity to commercialize hydrogen fuel cells.

Question 2: Approach to performing the research and development

This project was rated **3.8** on its approach.

- Two-pronged approach with data collection – analyze miles driven and performance of fuel cells.
- The project is well-integrated and supportive of other technology validation efforts.
- Very good.
- The approach is well though out and comprehensive and will certainly lead to accomplishing the objectives.
- The direct comparison to diesel buses is well done and appropriate.
- Built using the same procedures that NREL is using for FCV projects. Work seems to be relevant and timely.
- Very good focus on key parameters – miles/kg, $/mile, maintenance costs, etc.
- Fleet data collection has many advantages to promote/focus FCV technology.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.8** based on accomplishments.

- Data collected is well analyzed and disseminated.
- Good progress during past year to collect data from multiple sites.
- While data is still being gathered, present analysis is good.
- Many excellent results have been obtained so far, particularly the complete final report for the VTA [Valley Transit Authority] demonstration.
- The project appears to be on track and progressing well.
- Project collects, organizes and reports data from bus operations. Hard to know how NREL could do this better.
- Very good charts showing performance of buses at three different sites.
- Highlights the benefits of hybrid design for fuel cell bus.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.5** for technology transfer and collaboration.

- Works closely and successfully with transit authorities.
- 4 fleets analyzed.
- Both diesel and fuel cell are analyzed side by side which provide excellent analysis for transit authorities.
- Excellent international collaboration through the IPHE.
- Good collaboration with transit agencies.
- Some international collaboration, with more planned.
- Excellent coordination with 4 fleets.
- International collaboration questionable.
- The extent of collaborations with domestic fuel cell and infrastructure providers was not fully discussed in the presentation. The international collaboration is good.
- Great interactions with international partners working on the same problem. A global strategy for data reporting is a useful outcome.
- Provide current status – where are they doing better on cost and performance?

Question 5: Approach to and relevance of proposed future research

This project was rated **3.3** for proposed future work.

- How to reduce the fuel cell economy?
- Project does not appear to have well-defined, long-term objectives with milestones and a clear end-point.
- More data will obviously increase work.
- Suggest international work be separated into its own project.
- Suggest future inclusion of other fleets.
- The proposed future work is appropriate to continue progress toward the project objectives. The potential for evaluating more fleets is being considered.
- NREL simply proposes more of the same. Makes sense to continue gathering these data. Others could do it, but NREL does it very well.
- Good plan.
- Please include data from previous cold climate bus operation (e.g., Chicago and Vancouver) if resources permit.

Strengths and weaknesses

Strengths
- Excellent collaboration with transit companies and international partners, reporting of results and dissemination.
- Qualified PI at NREL.
- Excellent analysis capability.

- Experience with handling confidential data.
- The evaluation is fairly comprehensive, including both vehicle and infrastructure data. Various fueling systems (hybrid, ice, fuel cells, etc.) are included. The baseline using diesel buses is appropriate.
- Good collection of key parameters – data evaluation and comparisons.
- Benefits of hybrid and CNG designs are important lessons learned.

Weaknesses

- Warm weather geographic performance of buses only.
- Project would benefit from clearer milestones and longer-term planning.
- Lack of data so far.
- One facet that hasn't been evaluated yet is climate variation. All evaluations done so far have been in warm to moderate climates.
- Identify opportunities for further improvements in fuel cell fund and system performance, life, and cost.
- Please include environmental benefits (SO_x, NO_x, and noise).

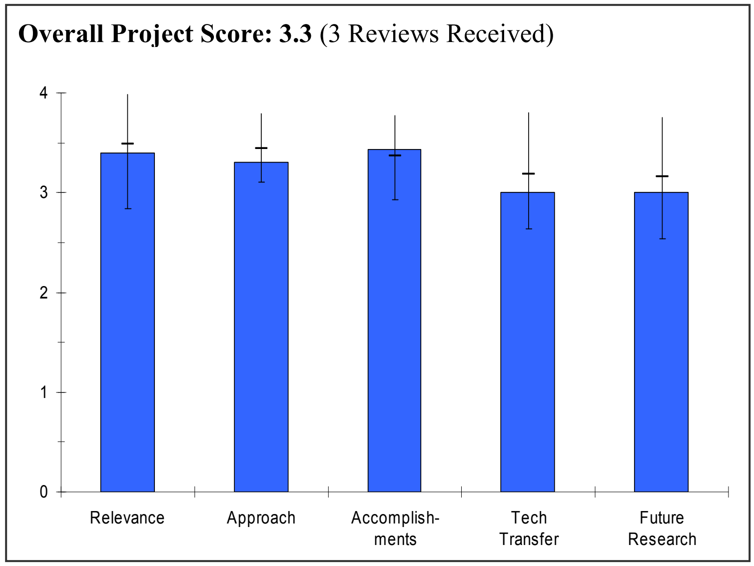
Specific recommendations and additions or deletions to the work scope

- Analyze the cost variations in more detail.
- Include cold climate performance such as Chicago and NYC if possible.
- None.
- Delete international component.
- Add more fleets in the future.
- Data from a cold weather climate would be valuable if added to the scope.
- Would be timely to hire a crew to make a documentary which describes these U.S. fuel cell buses. That needs to include rider interactions, maintenance experiences, and other stakeholder inputs. That DVD could be very timely data as other cities consider transit options.
- Compare U.S. data with European and Japanese counterparts. Rationalize the differences and identify the opportunities.

Project # TVP-02: Geographically Based Hydrogen Infrastructure Scenario Analysis
Margo Melendez; NREL

Brief Summary of Project

The overall objective of this project is to identify the best infrastructure scenarios to meet key transition scenarios and to identify implementation issues in the 2015-2025 timeframe. Two of the scenarios being looked at in 2025 are: 5 million vehicles and 4,000 refueling stations in 2025, and 10 million vehicles and 8,000 refueling stations. Several urban areas have been analyzed to determine the number of hydrogen refueling stations needed and the percent of the population that would be served.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.4** for its relevance to DOE objectives.

- Supplies DOE with information on size of minimum societal effort needed to support assumed projected H2 vehicle penetrations.
- This project supports DOE's goals for infrastructure development.
- This shows the feasibility and one possible scenario for establishing a hydrogen fueling infrastructure to support the hydrogen economy.
- This analysis, when combined with other analytical initiatives, will provide valuable insights for consideration during development of Federal policies to support hydrogen commercialization.

Question 2: Approach to performing the research and development

This project was rated **3.3** on its approach.

- Good use of data from existing gasoline infrastructure, vehicle use, and lifestyles; all evaluated with GIS overlays.
- This project uses the HyTrans model to develop estimates for the number of hydrogen stations needed for early adoption in a phased approach.
- Well integrated with other DOE-funded modeling and analysis activities.
- Existing databases are utilized in a logical and readily understandable manner.
- Is not R&D.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.4** based on accomplishments.

- Project is nearing completion with lots of useable information for policy makers and business planners on refueling infrastructure needs.
- The sources of data and transparency of assumptions and technique will be helpful as others begin to use this data.
- The technical value has been accomplished at reasonable cost.
- Provides a limited rollout plan by state.
- The results are laid out in a methodic and easy to understand manner.

- Provided sound underpinning and results for a required DOE report to Congress.
- Work has essentially been completed in a timely manner.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- Capabilities of ORNL and NREL investigators appear to have been successfully paired.
- N/A – no information available to determine this category.
- I know there has been collaboration but nothing is shown.
- Results of analysis shared with many parties of interest at multiple workshops.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- Work exposes the need to consider different refueler deployment patterns for different metropolitan areas; e.g. LA has demand for more even distribution compared to major radial corridors found in NY and Chicago.
- None.

Strengths and weaknesses

Strengths
- Uses publicly available Government held data as its basis and is used in an open transparent analysis. This is useful as a comparison to projections made by oil companies in prior years.
- The data output from this project offers considerably greater information about the needs and the land use changes (options) needed to introduce such a pervasive new infrastructure.
- Good phased approach which supports the DOE MYPP goals and targets for infrastructure.

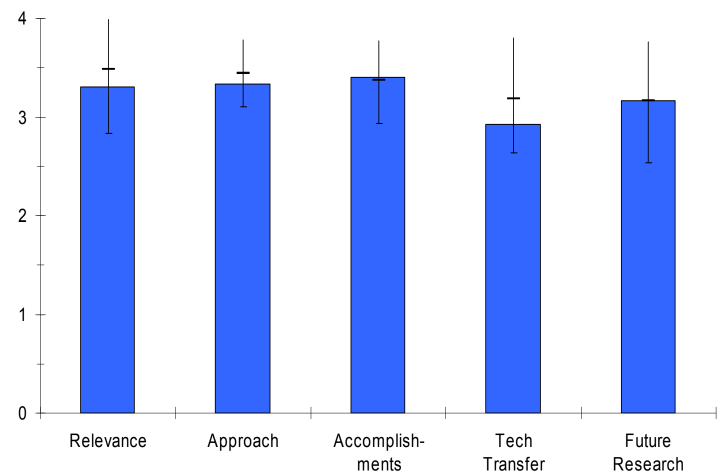
Weaknesses
- Attempts to project minimum required infrastructure using data developed and responsive to the highly developed I.C. engine and gasoline delivery methods.
- FCV introduction and initial uses may differ markedly from the spectrum of vehicle needs serviced by existing fueling infrastructure. Therefore, reliance on existing data may not be as solid as is typical.

Specific recommendations and additions or deletions to the work scope

- Here's a test: would this methodology, if used to show gasoline station growth, have predicted multiple gas stations on busy intersections?
- Compare oil company projections for minimum needed infrastructure with these results; do they show agreement?
- Use this information to project potential impact on existing energy infrastructure needed to supply these energy intensive users; i.e., impacts on local natural gas and/or electricity supplies and physical distribution assets.
- More information should be provided on how the data was developed. What was the methodology?
- Similar work to update these results should be undertaken in two or three years.

Project # TVP-04: Policy Options for Hydrogen Vehicles and Infrastructure
Steve Lasher; TIAX

Overall Project Score: 3.3 (4 Reviews Received)



Brief Summary of Project

The objective of this project is to identify and evaluate policy options to support the introduction of hydrogen vehicles and infrastructure. Policy options were grouped according to whether they were early-transition, late-transition, or commercial stage. They will next consider:
1. Could it be legislated and implemented?
2. Does the magnitude of the incentive make a difference?
3. How would the incentive affect other fuels and industries?

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

- Evaluation of potential impact of a variety of policies to accelerate adoption of hydrogen-fueled vehicles is a useful exercise.
- This supports DOE's goals.
- Useful for a review of policy options for acceleration of fuel cell vehicle markets.

Question 2: Approach to performing the research and development

This project was rated **3.3** on its approach.

- Reasonable evaluation of conventional policy options.
- Analyzed DOE's phased approach as outlined in the MYPP.
- Short duration and small project, but with considerable output.
- Is not R&D.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.4** based on accomplishments.

- Completed work as planned.
- Clearly reported results.
- Hood analysis reported in an easy to understand way.
- Completed study.
- This low-budget task was completed quickly. It contributed to scenario analysis activity led by NREL, and to establishing a baseline perspective on policy options.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.9** for technology transfer and collaboration.

- Incorporation of additional experts from the financial industry would have enhanced the project (recognizing that the funding was so small that this is probably not a practical suggestion).

- Unclear how collaboration occurred.
- Project supports DOE, with little other collaboration.
- The work used and contributed to other analytical initiatives and models.
- Results of this work were shared with many parties of interest at multiple scenario analysis workshops.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.2** for proposed future work.

- More creative incentives, rather than rehashing former (and mostly failed) incentive programs for other fuels, should be proposed.
- None.
- Work was completed.
- No future plans were discussed.
- Work completed. No follow-on proposal.

Strengths and weaknesses

Strengths
- Easy to understand results provided supports DOE's phased approach to infrastructure development.

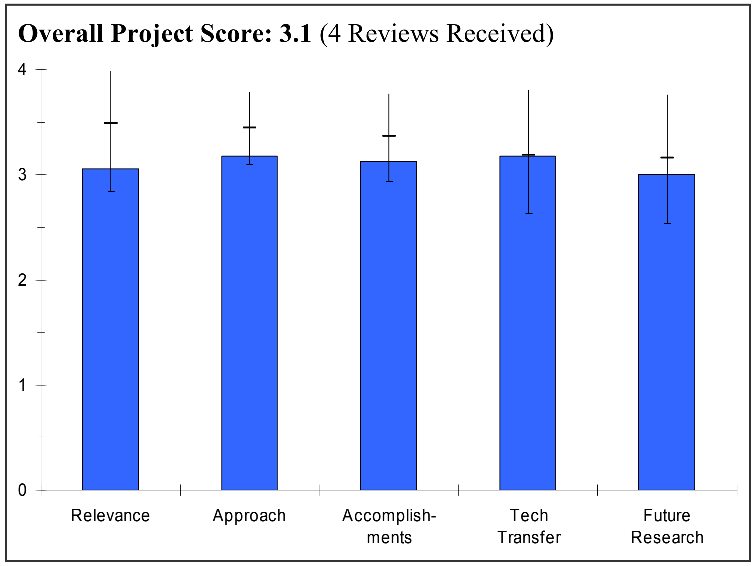
Weaknesses
- Depth of the analysis is insufficient (but so was the funding).
- Suggested that model used for ethanol could be useful for fuel cell infrastructure. Results are qualitative. Little discussion about previous vehicle mandates such as earlier US CAFE mandates or the CA ZEV mandates. No discussion about subsidies for customers, which might be a better option than continued OEM subsidies. Should include comparisons with the multibillion subsidies recently given to nuclear industry and other subsidies (including liability insurance) by the Congress. Also, a study of total subsidies including State and Federal that the auto industry receives today would be of interest, with the idea that fuel cell systems would require only a small fraction of such benevolence.

Specific recommendations and additions or deletions to the work scope

- None.

Project # TVP-08: Hydrogen Filling Station
Rick Hurt and Yitung Chen; UNLV

Brief Summary of Project



As a first step in the development of a hydrogen utilization network, the University of Nevada-Las Vegas Research Foundation is installing and analyzing the performance of a hydrogen generating and fueling system powered by solar energy. Objectives include development of generation and fueling system requirements, survey of potential sites for the filling station and determining favorable/unfavorable characteristics of each, selection of the site with site plan and support to the site permitting process, design of the system layout, construction of the filling station in Las Vegas, monitoring operation of the system, and characterizing its performance. In the second step of the process, the filling station is being supplemented with a high-pressure electrolyzer that was developed for this project. Two utility vehicles are being converted to use hydrogen as fuel. One of these is an electric vehicle that will function as a hybrid full cell vehicle; the second is a hydrogen-fueled internal combustion engine system converted from a gasoline-fueled ICE system. Finally, engineering and performance demonstration of tandem solar cell systems is taking place as well as some basic science studies.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.0** for its relevance to DOE objectives.

- This project is introducing hydrogen and renewable resources safely and with many personal interfaces to a broad spectrum of the community.
- Project covers many aspects of the Hydrogen Program's portfolio
- Direct application to H_2 generation and refueling.
- This project is useful; however it does not support the DOE's large effort to demonstrate fuel cell vehicles and infrastructure fueling.

Question 2: Approach to performing the research and development

This project was rated **3.2** on its approach.

- Using a university associated team as a basis for broader collaboration with the local community to introduce hydrogen applications is an approach trusted by society.
- The project is designed to be both flexible and inclusive of new community partnerships.
- Large overall program with many small projects – need better coordination/integration.
- Good focus on high pressure electrolysis.
- Good focus on vehicle conversion and demonstration.
- The emphasis on renewable energy sources is interesting. The hydrogen production capacity is far larger than the projected demand.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.1** based on accomplishments.

- Community involvement and enthusiasm is proof of the positive accomplishments produced by this project.
- Consider that the project has already successfully engaged the local water district (who now offers use of their land, as well as management capabilities), a local developer of a photochemical water splitting technology, a local automotive and marine service company, the local power company (who provided the design and hardware for the generator electrical interconnection), and others.
- The amount of local resource support for this project far exceeds the nominal 20% cost share officially ascribed to this project.
- All projects seem to be making progress, but hard to tell if they are on target.
- Coordination/integration is not clear.
- Should focus more on photoelectrochemical progress and scale ups.
- The electrolysis system is operational. Good effort to educate UNLV students, professors, school teachers, and others. Useful website up with all production data available.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.2** for technology transfer and collaboration.

- This project is bringing hydrogen applications out of the protected environs of structured "projects" and into the everyday lives of various members of the community, and doing so in a safe, technically supervised manner.
- Good project partners.
- Should coordinate with large auto and DOE groups.
- Biggest collaboration appears with a vendor.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- Once technology opportunities are guided into the hands of the everyday community, innovation will certainly result.
- Should focus on completing hardware and then refueling demos.
- Project appears to be in final phases and future plans are not clear.

Strengths and weaknesses

Strengths
- Solid core of technically competent sponsors.
- Visible solar energy user and producer of hydrogen in a solar rich resource area.
- Multiple community access points.
- Project is sufficiently stable and trusted to have attracted additional local resources; e.g., the water department enthusiasm and resources.
- Team appears to have strong R&D technology capability for areas under investigation.

Weaknesses
- Hard to tell if individual projects are contributing.
- Overall integration of all the projects is not clearly portrayed.
- Team is weak in established manufacturing capability.
- UNLV needs to get some hydrogen consumption to match their production capacity.

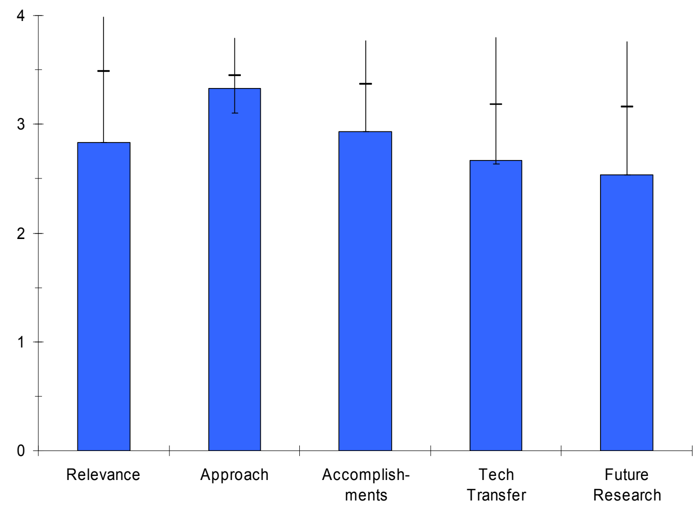
Specific recommendations and additions or deletions to the work scope

- Far too much material presented.
- Presentation/poster much longer than "allowed" and still does not provide sufficient detail on most projects.
- Should be multiple presentations, including one that specifically addresses how all the others are integrated into a sensible, focused program.
- Add main auto company to team.
- Seems an obvious site for a Federal fuel cell bus demo project.

Project # TVP-11: Florida Hydrogen Initiative
Ed Levine; Florida Hydrogen Initiative

Brief Summary of Project

Overall Project Score: 2.9 (3 Reviews Received)



The Florida Hydrogen Initiative (FHI) is a non-profit organization incorporated under the laws of the State of Florida to move Florida to the forefront of the nation's hydrogen economy. The Florida Hydrogen Initiative uses its resources to aid the development of a robust Florida-based hydrogen industry thereby establishing Florida as the cornerstone of a southeastern hydrogen hub. The non-profit corporation is comprised of public leaders, university researchers, citizens, and industry representatives. The Florida Hydrogen Initiative, Inc. develops Florida's Hydrogen Infrastructure by:

- Brokering partnerships for applied technology demonstration projects throughout the state;
- Sponsoring research in the production, storage and use of hydrogen fuels;
- Facilitating technology transfers between the public and private sectors to create, build and strengthen high-growth potential, technology companies.

Question 1: Relevance to overall DOE objectives

This project earned a score of **2.8** for its relevance to DOE objectives.

- Set of small focused projects that address specific barriers to a hydrogen economy
- This is 3 unrelated projects with some more relevant than others. Distinctions need to be clearer.

Question 2: Approach to performing the research and development

This project was rated **3.3** on its approach.

- Each project has a reasonable plan.
- Approach on citrus residue conversion should investigate use of bad crops and weather damaged crops, as well as peels.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.9** based on accomplishments.

- All projects are making progress.
- Project timing versus status of development wasn't clear.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.7** for technology transfer and collaboration.

- Good teaming effort.
- Creative outreach efforts.
- No evidence was noted.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.5** for proposed future work.

- Plans are logical.
- Mr. Levine plans to follow up with DOE staff and managers of other DOE projects. It is clear that he desires to accomplish the tasks in this project so that they contribute as much as possible to helping achieve goals and objectives established for the DOE hydrogen program.

Strengths and weaknesses

Strengths
- Three good ideas are evident.

Weaknesses
- Completion of all three projects is totally independent and basically unrelated.

Specific recommendations and additions or deletions to the work scope

- The traveling museum should tie the other projects into one story with ties to the general topic of hydrogen.

2007
Safety and Codes & Standards
Summary of Annual Merit Review Safety and Codes & Standards Subprogram

Summary of Reviewer Comments on Safety and Codes & Standards Subprogram:

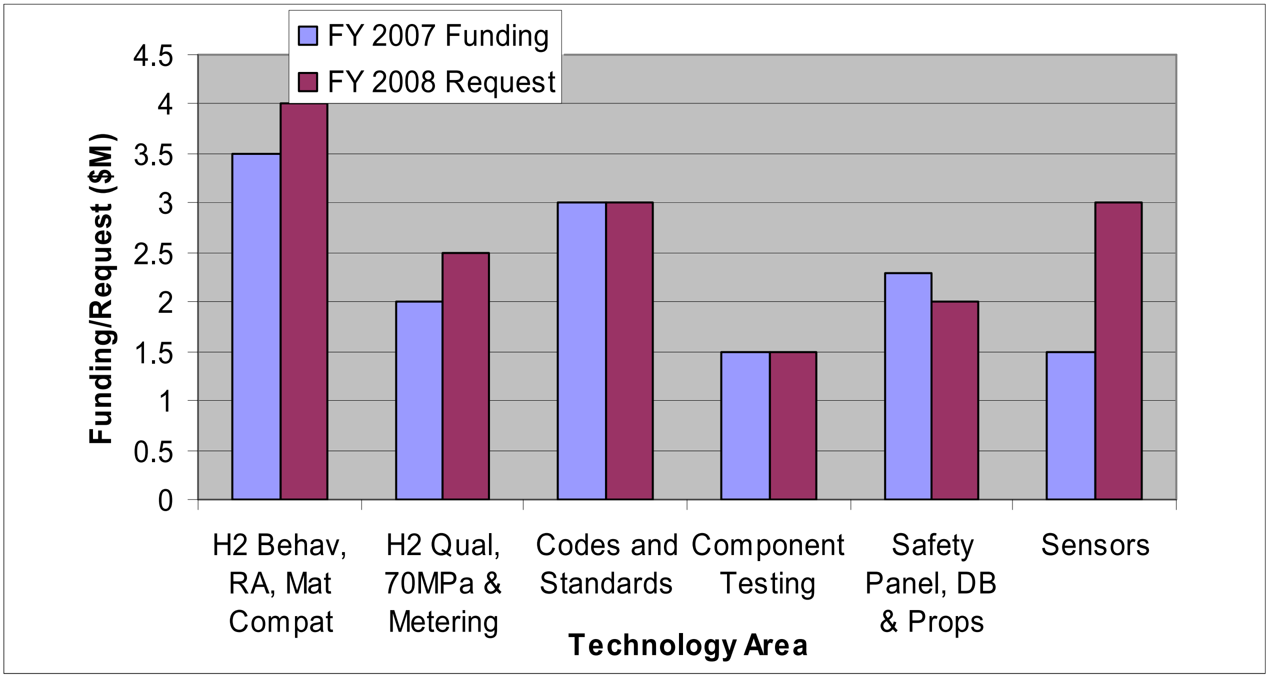
In general, Safety and Codes and Standards Subprogram reviewers stated that projects were productive and successful. The Reviewers were impressed by the breadth of activities and the ongoing commitment to safety, codes, standards and information-sharing activities. They stressed that successes in this subprogram touch every other DOE hydrogen-related activity by fostering acceptance, collaboration and communication with critical stakeholders.

Reviewers stressed the importance of continuing efforts in critical areas such as hydrogen materials research, hydrogen codes, standards and permitting materials coordination efforts, hydrogen quality, and safety incident reporting and best practices. Suggestions for maximizing progress included leveraging the efforts of universities, standards organizations, national labs, complementary government agencies, and industry.

Six safety projects were reviewed. The Hydrogen Materials Research and Development project is focused on materials research to support the development of technically sound codes and standards to ensure the safe design of infrastructure for the storage and transport of high-pressure hydrogen gas. The project was praised for excellent collaboration with industry and SDOs and CDOs. Reviewers noted that the public availability of the data obtained from this project was especially invaluable. It was suggested that new materials should be tested and system-level as well as component level tests should be explored. The Hydrogen Incident Reporting Database and Hydrogen Safety Best Practices Website were considered to be valuable tools for the future implementation of hydrogen infrastructure. More interaction with other safety organizations and a careful examination of the scope of the best practices website were encouraged. The Hydrogen Codes, Standards, and Permitting Materials work was praised for its varied engagement with industry, government, and researchers, particularly national laboratories. It was noted that hydrogen codes and standards work could benefit from greater focus in the future. However, hydrogen fueling station permitting activities were seen as progressing well. Hydrogen quality work was praised for its strong collaboration with a broad spectrum of stakeholders worldwide. Some reviewers pointed out the need to generate data in a timely manner and to work more with SAE and with state hydrogen programs. The Hydrogen Safety Panel was regarded as a strong concept with qualified membership. Fostering the collaboration and communication of safety experts has helped to promote and ensure safety across hydrogen-related projects. The number of safety plans reviewed was considered impressive. It was recommended, however, that Panel membership be rotated to disseminate knowledge and broaden the experience represented on the Panel. The final Safety, Codes and Standards project on intelligent optical sensors, however, received lower than average reviews. Although the project was deemed relevant to DOE program goals, the project may have difficulty overcoming technical barriers and could benefit from outside collaboration and a commercialization plan.

Safety and Codes & Standards Funding:

Safety and Codes and Standards funding includes international activities as well as national development and coordination among several agencies. While funding had been a major concern in previous years, this fiscal year, the subprogram received full funding. In particular, progress in the area of hydrogen quality was considered a consequence of increased funding over last year.



Majority of Reviewer Comments and Recommendations:

Subprogram scores were average to high, with an overall average of 3.3. Reviewers also indicated that the Safety Panel has a range of high quality representatives but the Panel should rotate its membership to stay fresh. The overall progress on Materials R&D was seen as impressive.

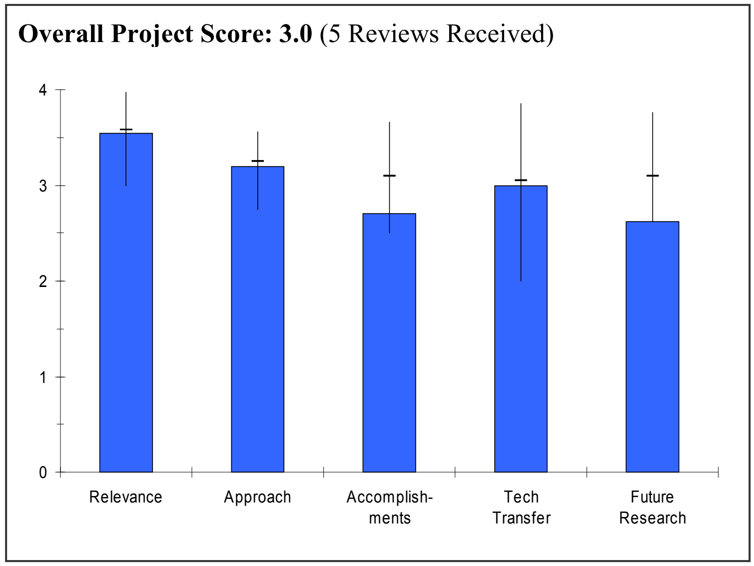
Because the Program received full funding this year, the distress over budget cuts that was seen in previous years was pleasantly absent.

Recommendations included:

- Expansion of the set of materials tested under the Materials R&D activity.
- Expansion of data generation for hydrogen quality work; ensure coordination with ANL's hydrogen quality working group.
- Increase collaboration with regulatory agencies, CDOs and SDOs, professional groups, and other federal agencies for the Hydrogen Best Practices Manual and Incident Reporting Database.

Project # SA-01: Codes, Standards and Permitting Materials
Jim Ohi; NREL

Brief Summary of Project



In this project, the National Renewable Energy Laboratory is working to implement a consensus national agenda on domestic and international codes and standards for hydrogen systems in commercial, residential, and transportation applications; facilitate permitting of retail hydrogen fueling stations in the U.S. through education and outreach to state/local code officials; establish requirements for hydrogen codes and standards based on scientific data, modeling and analysis; and enhance DOE's role in the development of International Standards Organization (ISO) and other international standards; and strengthen consistent and sustained representation by U.S. government and industry at international standards forums. This will be accomplished by bringing together experts to address key issues, coordinating collaborative national and international efforts between government and industry, and by serving as the central point of contact for up-to-date information on codes and standards activities.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

- The project is critical to safety and safe deployment of the hydrogen economy.
- Safety is critical to commercialization.
- There is some overlap between some of the groups sponsored under the codes and standards activities.
- There is some overlap with DOT activities in vehicle safety.
- The C&S effort is always looked at as being a building block for the hydrogen economy.
- Safety, codes and standards will be necessary for a smooth transition to a hydrogen economy.
- National Template is a good initiative to coordinate OEMs.
- This project is highly relevant, if not critical, to the success of the Hydrogen Fuel Initiative.

Question 2: Approach to performing the research and development

This project was rated **3.2** on its approach.

- The project identifies research gaps.
- The project facilitates research programs and partnerships between national laboratories, industry, and government.
- The project in some ways focuses not so much on technical barriers as on policy or harmonization barriers.
- The project has an overall plan that it is following. This is a difficult and multifaceted topic which needs a plan that spans years.
- Wide-ranging approach requires strong management
- Good approach to R&D.
- A R&D timeline needs to be presented.
- The approach on hydrogen fueling stations appears sound and was presented in sufficient detail.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.7** based on accomplishments.

- Facilitates coordination between Codes and Standards Development Organizations through FreedomCAR, Hydrogen and Fuel Cell National Coordinating Committee, Hydrogen Safety Panel.
- Progress has been good in this area and has come a long way over the last few years. Good progress this past year as well.
- Progress on using composite vessels in DOT and ASME applications is continuing to lag, but it looks like there is a lot of effort on tanks this next year.
- Accomplishments and progress lack depth.
- Good progress relating to hydrogen compatibility.
- Need to work also with state agencies relating to familiarity.
- Very good progress on HFS work.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- Close coordination particularly among national laboratories.
- The project interfaces with multiple organizations.
- Drop testing needs to be validated.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.6** for proposed future work.

- This effort is more of a forum for sharing information and collaborating on research planning, but not on research supporting all codes and standards activities.
- Future component work seems very focused on tanks, hopefully not to the detriment of other important pieces.
- Future direction is lacking in focus.
- Not very descriptive related to proposed future research.
- Are these the critical items that need to be addressed in the next year?

Strengths and weaknesses

Strengths
- Large number of participants, cross-cutting industry, government, researchers
- Project is providing overall path for C&S activity to monitor and identify areas that need assistance. The PI is knowledgeable about the effort.
- Important topic, engaging industry.
- An experienced team.

Weaknesses
- Some overlap between subgroups, and Standard Development Organizations working independently anyway.
- The project can only influence rather than drive standards process.
- Program is lacking in focus.
- Substantial goals or milestones are lacking.
- Need to engage the right stakeholders.
- Choice of words for describing.
- Very ISO focused.

- Slide 3, Approach: Program Structure, should be updated to more appropriately reflect safety portion of the overall program.
- This project covers a lot of ground with many facets and interactions with other parties, but I did not get a sense of what the critical areas that require attention/action over the next year are, for example. Consider approaching the presentation in 2008 in this manner.
- Provide all slides to reviewers prior to the meeting. I was surprised to be reviewing a second part to the presentation.

Specific recommendations and additions or deletions to the work scope

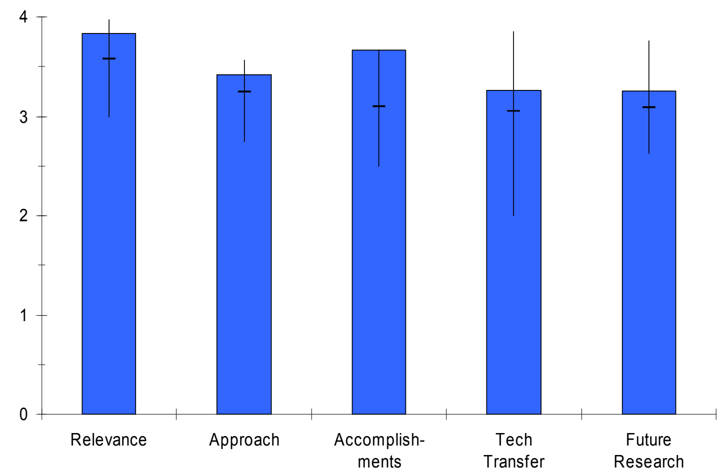
- None. The scope may be too broad at this time, but better to have some overlap and a broad scope if resources permit during this developmental stage.
- Provide funding to industry partners to accelerate standards development, improve quality, and increase efficiency of process. These standards processes are on a volunteer basis and it takes years due to infrequent/inconsistent activity.
- The project could help resolve internal differences within different divisions of DOT (e.g., NHTSA/PHMSA) with respect to the use of composite vessels.
- Focus on a study for hydrogen release while engaging industry expenses.
- Help direct NCMS projects related.
- Review future work plans with Tech Team before implementation.
- I suggest developing a pictorial representation(s) of the material shown on the slide entitled Technical Progress: Information Repository Concept. I found the slide difficult to follow.

Project # SA-02: Hydrogen Materials R&D
Brian Somerday; SNL

Brief Summary of Project

To ensure safe design of structures for storage and transport of high-pressure hydrogen gas, this project is focused on acquiring material property data that reflects service conditions. Sandia National Laboratories will identify and document existing data on hydrogen compatibility of materials from technical journals and reports, and then generate new data through materials testing, emphasizing testing in high-pressure hydrogen gas. The project provides advocacy and technical support for the codes and standards change process.

Overall Project Score: 3.5 (6 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.8** for its relevance to DOE objectives.

- Materials compatibility data are needed for deployment of infrastructure.
- This is the basic information that is required to roll out the technology to support the hydrogen economy. This work will not be funded privately, and if it were, would be proprietary.
- Materials compatibility is key to safety and the implementation of codes and standards.
- Very relevant program for Codes and Standards.
- Very important project for accomplishing the Hydrogen vision.
- This project is highly relevant to the success of the Hydrogen Fuel Initiative.

Question 2: Approach to performing the research and development

This project was rated **3.4** on its approach.

- Sharply focused on testing.
- Sharply focused on providing comprehensive technical reference.
- The approach is excellent and the Tech Reference guide is an excellent resource and repository of information.
- Good involvement of SDOs and industry for testing.
- Good approach relating to initial work.
- Approach is good, but should also consider composites, low carbon steels, and other materials beyond stainless, copper, and aluminum.
- The overall approach is very sound, combining experimental work, collaboration with "external" groups such as ASME and collaboration with "internal" groups such as the DOE Pipeline Working Group.
- An excellent approach for making information available more broadly through the web-based technical reference.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.7** based on accomplishments.

- Completed volume 1 of Technical Reference.
- Completed a lot of testing.

- Generated benchmark cracking thresholds.
- Developed test robust procedures.
- Progress could be faster, but the project speed is understandable. The progress is still excellent.
- Good initial set of materials.
- Excellent progress including new glove-box testing.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.3** for technology transfer and collaboration.

- The Technical Reference consolidates materials compatibility data for all industry stakeholders.
- It appears that Sandia is very responsive to partners and actively seeks input on approach and priorities.
- Good collaboration across industry and with codes and standards organizations
- SNL has taken their results and published, given to standards organizations
- Good coordination of materials testing with Pipeline Working Group, but that data should also be included in materials database.
- Several aspects to the collaboration which appear to be well thought out.
- I assume that collaboration with industrial gas companies and others experienced with handling hydrogen is through the ASME collaboration.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.3** for proposed future work.

- Plan's continuation of testing materials builds on past efforts.
- Plan's augmenting publication of technical references.
- There is a plan laid out for FY08 and it shows good progress on issues that are important to the hydrogen economy.
- Future work clearly builds on past accomplishments.
- Very clear plan related to present and previous R&D activity. However, future plan needs to be better defined.
- Comments made by others regarding component testing, weld-related work should be considered.
- I would ask myself the question whether the community that will benefit from access to and knowledge of this work is fully aware of the work; consider other communication mechanisms as appropriate.

Strengths and weaknesses

Strengths
- Generating valuable data set for deployment of infrastructure.
- Performing basic work that no one else is doing, and will help the entire industry equally. If done independently, the work would be private and not as readily available.
- Answering questions that have been out there for years, but no one had the resources to test.
- Very impressive progress.
- A systematic, analytical approach to materials compatibility.
- Technical expertise of staff involved and results achieved as noted in the S,C&S award.
- An excellent presentation.

Weaknesses
- None.
- The tests are time consuming, so limited data can be generated in one year. This also makes it difficult to fully evaluate all the variables which could affect results.
- Fatigue testing can't effectively evaluate or speed up time-based issues that might occur over years.
- Need to coordinate closer with pipeline materials working group.
- Component-level testing / understanding of system effects not known.

Specific recommendations and additions or deletions to the work scope

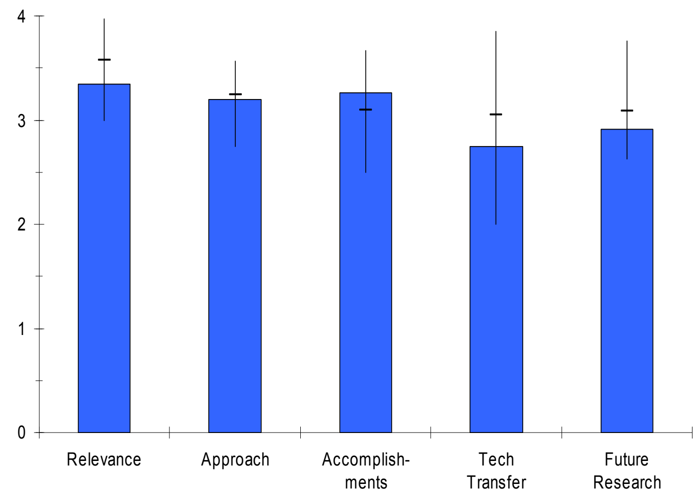
- None.
- Additional materials should be added beyond stainless steel.
- Increase support for this effort in order to meet standards timeline.
- Survey industry regarding new materials.
- Explain who they mean by "materials work."
- Consider adding other materials beyond stainless, aluminum, and copper.

Project # SA-03: H_2 Incident Reporting Database and H_2 Safety Best Practices Website
Linda Fassbender; PNNL

Brief Summary of Project

The objectives of this project are to 1) establish a web-based system for open sharing of lessons learned from hydrogen incidents and near misses through use of a confidential reporting tool for such safety events; and 2) provide a Hydrogen Safety Best Practices resource to enable widespread benefit from the wealth of knowledge and experience already attained in industry, aerospace and elsewhere.

Overall Project Score: 3.2 (6 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.4** for its relevance to DOE objectives.

- The incident database is a good support system for encouraging cross-learning among various DOE funded programs.
- The best practices website could be useful to certain organizations new to working with hydrogen and not familiar with existing literature. Caution should be exercised in characterizing the purposes of both websites, the intended audiences and uses, and the context of the information available.
- Real-world safety performance data collection is critical to deployment of the hydrogen economy.
- Providing single-point resources for sharing lessons learned and best practices will be beneficial in the safe implementation of the hydrogen economy.
- An important contribution to hydrogen safety.
- Although hydrogen is used widely, and hydrogen safety is well-established in the hydrogen industry, the ability to move safe practices to a larger user group will enhance safety when hydrogen usage increases across many sectors. This argues strongly for this project's importance.
- There is relevance for this project to support the Hydrogen Fuel Initiative. I have reservations as to the utility of this project as presently configured. However, small changes in scope and direction may relax my reservations. They will de discussed below.

Question 2: Approach to performing the research and development

This project was rated **3.2** on its approach.

- Development of the Best Practices website should advance in cautious and close coordination with entities within the codes and standards and regulatory communities. These organizations historically house best practices within standards, codes, regulations, and other published documents.
- The DOE Best Practices website should limit it's scope to cover a summary of high points of available practices from published, standards, codes and regulations (and other relevant published documents), by subject area, to act as a guide to official literature and a link to relevant captured incidents.
- Straightforward approach. Collect incident and best practices data and disseminate through publicly available website.
- A good process has been set up to capture hydrogen incidents and develop lessons learned.
- Good plan for best practices.
- The research methods used appear to be thorough and reliable.
- The data sources appear to be appropriate.

- It is recommended that all potential data sources be used including NFPA, NASFM, DOT, UL, Factory Mutual, Insurance Companies, and other industry data bases. Inclusion of these data sources may contribute additional data.
- The approach adopted for this project appears sound.
- Expanding the search and report function to leverage synergistic industries by incorporating fuel gas (natural gas) and industrial compressed gas incidents and best practices will help address best practices and generate a list of common escapes that then can be addressed by training.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.3** based on accomplishments.

- The structure of both websites is clean, easy to read, and well structured.
- Capturing even 10 incidents from last year's programs is an excellent accomplishment.
- Search features will be very useful to program participants and site users.
- 130 incidents to date.
- The website receives several thousand hits.
- Technical accomplishments seem modest.
- H2 incidents website is up and running.
- Best Practices is under development.
- There was a recent change of leadership. The new leadership has grabbed the ball.
- Good progress shown by implementing incident reporting website.
- Process for handling incidents appears to be well thought out.
- Review of Best Practices by Hydrogen Safety Panel is a good way to ensure technical accuracy and relevance – this is a strength.
- Long length of project might be inconsistent with moving to commercialization. Who will do this when DOE stops?
- The progress appears to be appropriate for the time and budget.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.8** for technology transfer and collaboration.

- In future reports, the project should report how it is linked with the Safety Panel, the Tech Val teams, and other program groups (interfaces, meeting frequency, feedback loops). The DOE program participants are both the primary audience/users, and (should be) the primary reporting parties into the incidents database – without proper and proactive coordination, the usefulness of the database will decrease.
- Data sharing through website.
- Appears that incidents are reported.
- Lessons learned/best practices/incidents linked.
- Linked to Hydrogen Safety Panel so that information here is transferred into safety assessments of DOE projects.
- Limited to date.
- In future, there could be more active collaboration with other safety organizations (OSHA, NFPA, NTSB, Fire Marshall's Association, etc.).
- Additional linkages to other DOE Hydrogen Safety efforts would be helpful.
- It would seem that this need will persist beyond the length of the project. Some technology transfer or collaboration with an organization who will take over this task for industry would be a valuable addition.
- The information transfer and collaboration activities are a good start.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.9** for proposed future work.

- As identified by another reviewer during the question and answer period, a timeline for the databases and websites should be developed including possible handoff/interface scenarios out in 2012 (e.g., handing off/working with the insurance, codes & standards, and regulatory communities who typically maintain this type of information for other industries/technologies).
- It was unclear about how “trends” information would be identified through the incident database, how that information will be reported and reviewed, and who will receive that information.
- User interaction will be a key future feature that is well worth pursuing. This capitalizes on the community learning strengths of both online tools.
- Ongoing data collection.
- Leads to identifying trends.
- Review, feedback from safety panel, and integrating incidents and best practices.
- Need to develop other useful initiatives after Best Practices is up and running.
- Continued improvement in data and reporting is included in the plans. This is a strength.
- The proposed future work is consistent with the present scope of the project.

Strengths and weaknesses

Strengths
- Making appropriate, non-proprietary, safety-relevant information available to DOE program participants.
- Encouraging interaction, continuous review and development, and communal learning among program participants.
- Real-world data collection is necessary.
- Project provides single-point resources for best practices and incident tracking.
- Web based – living documents.
- Right topics.
- Website dissemination.
- Comprehensive effort.
- Review by Hydrogen Safety Panel.
- The project heavily leverages the existing hydrogen infrastructure which is based on industrial practices and OEM procedures, which are much less cavalier than the practices used in synergistic industries, which follow commercial practices and/or public usage.

Weaknesses
- If the incident website is identified by high-profile first responder and other outside-of-industry stakeholder groups, the information available could be taken out of context (lab/research incidents vs. real-world incidents). Appropriate language should be clear and upfront on both websites to characterize the primary audience, context of the information, and scope of available information.
- Adding some type of time-related signature to each incident report would be useful to identify learning trends and track the frequency of related incidents over time. If specific timing/date information is considered sensitive, perhaps more general time stamps can be pursued.
- There may be some overlap with best practices developed by CDOs and SDOs.
- Change of management.
- Probably has been underfunded in past.
- There could be better collaboration with other hydrogen safety programs.
- Need some sort of transition to a commercial entity to handle this for the industry beyond the DOE funding timeline.
- The project does not explore the synergistic industries such as the natural gas and the compressed gas industries. Many of the more common occurrences that probably occur with usage by the general public would not be expected to be reflected in the data from safety sensitive industrial practices. The safety guidelines used by people trained for handling bulk quantities is more restrictive then the practices of the general public working with much smaller quantities.
- I am concerned that this activity will be perceived and marketed as hydrogen is a more dangerous fuel as compared to natural gas and petroleum.
- The collaboration for data does not appear to leverage all the existing incident reporting structures.

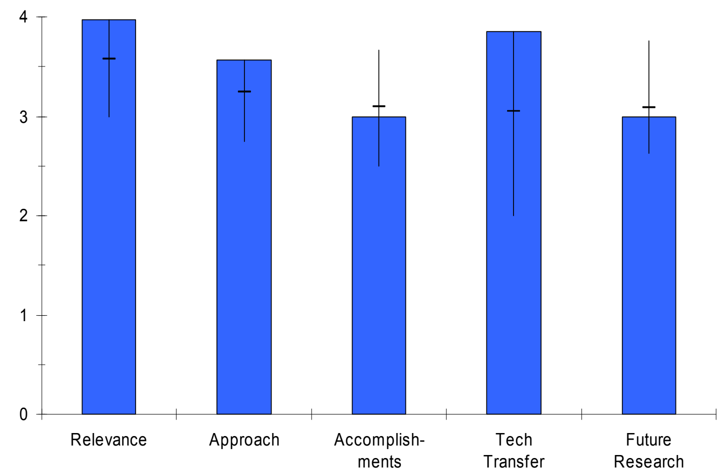
Specific recommendations and additions or deletions to the work scope

- The scope of the Best Practices website should be carefully considered in consultation with relevant government regulator agencies (e.g., OSHA), Codes & Standards Development Organizations (e.g., CGA), and professional groups (e.g., NASFM) who have traditionally published guidance information. The most useful outcome is that the Best Practices website helps summarize, at a high level, basic practices, links users to existing established information, and links each subject area to relevant captured incidents.
- Interfacing with the Tech Val program to understand if the 10 captured incidents are representative of all incidents or if they represent only a subset (indicating that some percentage of incidents are not being reported); in the case of the latter, barriers to reporting should be identified and addressed.
- None.
- DOE should nurture it and keep it well funded.
- Develop longer term plan with new initiatives.
- Consider a separate CNG incident database (rationale: hydrogen tanks and components are very similar to those of CNG. There is a much larger population available, which can provide quantitative failure rates).
- Implement an RFP, RFQ, or other methodology for partnering with industry to move this function into mainstream industry. Similar work is done by many, many industries, and should be done with hydrogen also.
- Expand the scope to include the natural gas and compressed gas usage. Specifically, including the natural gas vehicle activities, compressed gas cylinder usage and LPG usage.
- Expand the data mining to other sources – for example, federal (DOD, DOL OSHA, DOT PHMSA, US EPA), state (Environmental Protection, State OSHA) and private industry (Commercial and Residential insurance).

Project # SA-04: Hydrogen Quality
Jim Ohi; NREL/LANL

Brief Summary of Project

Overall Project Score: 3.4 (4 Reviews Received)



The National Renewable Energy Laboratory (NREL) is conducting research and development (R&D) and testing in support of national and international codes and standards efforts in the area of hydrogen fuel quality. Overall objectives are to collect, evaluate, and report assemblage of data and information, and to recommend hydrogen fuel quality specifications. In addition, NREL is developing consensus on critical analytical methods and procedures needed to verify recommended maximum levels of contaminants; forming two sub-teams to focus separately but iteratively on single-cell testing (performance-durability) and fuel cell system and fuel infrastructure engineering requirements and costs; and forming a modeling sub-team to develop and apply an empirical model to focus testing and enable projection of test results.

Question 1: Relevance to overall DOE objectives

This project earned a score of **4.0** for its relevance to DOE objectives.

- Very relevant, as evidenced by funding increase and good use of critical partners.
- Hydrogen purity is a very important parameter to rolling out hydrogen as a fuel. It is currently a very controversial topic that needs to be resolved and is potentially a roadblock unless all stakeholders agree on an approach.
- Hydrogen fuel quality is critical to success of hydrogen economy.
- This task is highly relevant to the Hydrogen Fuel Initiative.

Question 2: Approach to performing the research and development

This project was rated **3.6** on its approach.

- Looks comprehensive; with international partners; good baseline chart.
- A purity standard is very important, but it's more important to get it right than to get it fast. The approach seems more geared toward getting a specification in place rather than a practical specification in place.
- The approach needs to consider cost, effectiveness, and frequency of testing methods as part of the process.
- The international approach is appropriate.
- Plan for testing impact of impurities is well thought out. Just need to bring a sense of urgency to the process.
- The approach is appropriate for generating an International Standard.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- Chart and graphs used in presentation showed great progress.
- The specification is moving forward, but barriers still exist on cost/verifiability.

- Not clear that He impurity targets are difficult to achieve if use LH_2 distribution to stations (or LH_2 step in forecourt as clean up; impact of He on fuel cell is being evaluated now – efficiency hit to be quantified.
- To certify or validate station performance, also need to measure fuel temperature and flow rate in addition to catching a canister sample for analysis.
- Composite test matrix plans should have target dates for completion (and those dates should reflect a sense of urgency).
- Please bring a sense of urgency to this work.
- The progress to date appears limited. It is assumed that this is paced on funding.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.9** for technology transfer and collaboration.

- Great collaboration with worldwide partners.
- The project has representation from a wide variety of stakeholders.
- Extensive collaboration network.
- Work with USFCC ensures broad-based applicability and guidance.
- Very nice plan for ISO support work laid out in presentation. Need a similar work plan for coordination with SAE.
- Create comparable slide for SAE (just like ISO slide) – showing earlier establishment by SAE of interim standard and continuing reconsideration of inert levels by the SAE group. ISO and SAE are really working together.
- The stated and imbedded collaboration is reflective of the current, active industry representatives.
- The lack of acknowledgment of the testing completed by JARI and funded by NEDO in support of this activity is disappointing.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- Future work is "data-driven." Good approach. Good integration with other labs and agencies.
- The project needs to put more emphasis on the ability to accurately and cost-effectively validate fuel quality at stations. A specification that is unverifiable at reasonable cost is not a help.
- Very nice plan for ISO support work laid out in presentation. Need a similar work plan for coordination with SAE.
- Create comparable slide for SAE (just like ISO slide) – showing earlier establishment by SAE of interim standard and continuing reconsideration of inert levels by the SAE group. ISO and SAE are really working together.
- The objective of the future research is limited and does not reflect the short-term needs of the industry but rather the longer-term, international viewpoint, especially that of Europe.
- The specific needs are to generate a domestic standard and verification test methods to support the Hydrogen Initiatives in states like California, Michigan, Ohio, New York, Florida, etc. These states adopt domestic consensus standards by law.

Strengths and weaknesses

Strengths
- Increased funding should help this program go a long way – much better than last year.
- The project is taking a scientific approach.
- Extensive coordination and input from the broad spectrum of stakeholders.
- The strength of this project is the international collaboration focused on a longer term event horizon.

Weaknesses

- The tendency might be to take purity to a "lowest common denominator," which could result in a more stringent specification than necessary. Gaining consensus will be difficult given the variety of interests involved.
- The final purity specification must be verifiable using practical processes and at reasonable cost.
- Particulates cannot be excluded from the process stream with existing connection technology. Including particulates in the specification is problematic.
- Seems to be a focus on ISO to the detriment of SAE. SAE 2719 has been approved. Furthermore, SAE is an international organization.
- Lack of timelines and a commitment to them.
- Lack of public data on hydrogen impurities in current hydrogen sources; for example, if CO is present at 1 ppm, NH_3 and H_2S might not even be issues, since their concentrations are essentially zero, but we need public data to show this.
- The weakness of this project is the lack of progress to comply with the state hydrogen programs, many of which are still following the original DOE schedule. This is specifically evident when observing activity in California, which by law requires a fuel standard by January 2008.
- This weakness is magnified when it is understood that other states copy or adopt the activities of California, often with out the caveats and variances.

Specific recommendations and additions or deletions to the work scope

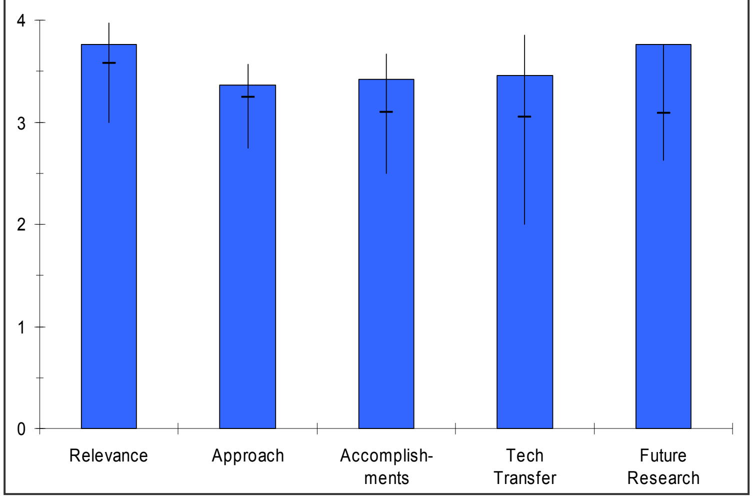
- Make sure that this work is consistent with, and complementary to, the AN-06 project being done by Romesh Kumar at Argonne.
- Expand research into making fuel cells more tolerant of fuel impurities as an alternate approach, or alternatively adding filtration equipment (e.g., fuel filter) to protect against damage.
- Dave Masten (GM) should be added to the North American Team membership.
- Continue to make data on hydrogen quality publicly available, or at least get a mechanism in place so that the Hydrogen Quality Task Force can get access to the data to guide the hydrogen impurity work.
- Accelerate these activities by eliminating the delays being encountered.
- Refocus the near term efforts to support the domestic agenda.
- Impart a sense of urgency to the parties involved in the data generation.

Project # SA-06: Hydrogen Safety Panel
Steven Weiner; PNNL

Brief Summary of Project

The Hydrogen Safety Panel supports the DOE Hydrogen Safety Program, focusing on the development and implementation of practices and procedures that will help ensure safety in the operation, handling and use of hydrogen and hydrogen systems for all DOE projects. Bringing together a broad cross-section of industrial, government and academic expertise, the panel provides expertise and guidance to DOE and assists with identifying safety-related technical data gaps, best practices, and lessons learned. Safety reviews focus on engagement, learning and discussion and are not treated as audits or regulatory exercises.

Overall Project Score: 3.5 (5 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.8** for its relevance to DOE objectives.

- Safety review of DOE funded projects is critical to the continuation of the Program.
- Safety is critical in research and demonstration programs.
- This project is critical to the continuation of the initiative and achieving the goals of the Hydrogen Initiative. One major incident could bring the Initiative to a sudden end.
- Anything that is done to accelerate the distribution of hydrogen safety knowledge will be beneficial to the Initiative.
- Safety is an important aspect of the Program.
- Outstanding project that is very important to Hydrogen vision.
- The near term effect of this activity is relevant to generating and disseminating safety guidance on projects support the Hydrogen Fuel Initiative.

Question 2: Approach to performing the research and development

This project was rated **3.4** on its approach.

- Providing safety review is a learning process.
- The expertise of the Panel membership is important to developing the approach for safety assessments and identifying gaps.
- The approach of focusing on priorities established by the Panel is very good.
- Not all of the barriers are being addressed to the extent that they could if funding were unlimited. Considering funding constraints, this approach represents a good balance.
- Safety reviews are performed in a way that brings considerably more knowledge to the process than would be achievable with out this activity.
- Focusing on safety plan content rather than format is very appropriate.
- Concept is good. I can only hope that the telephone interviews are effective.
- Realistically, the approach being taken is the only viable option.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.4** based on accomplishments.

- Safety panel reviews of DOE projects.
- Review of NREL data templates.
- Providing guidance and input to safety plans, practices.
- Conducting 23 safety reviews and reviewing 50 safety plans is pretty impressive.
- Responses from 147 projects on this year's two new questions is phenomenal and represents a wealth of information that will soon be available to the community.
- I guess the real measure of progress is the lack of serious hydrogen incidents. So, the panel is succeeding.
- Process appears to be working very well with several project plans have been reviewed.
- 2007 Safety questionnaire question "...the potential to result in the worst consequence" can be leading and there is no metric identified. Question should probably be eliminated.
- Accomplishments appear to be consistent with funding.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.5** for technology transfer and collaboration.

- Transfer/collaborations through diverse membership.
- Transfer between panel members and principal investigators.
- Transfer between Panel and H2 Incident Reporting and Best Practices, which ultimately provides a broader audience.
- When looking at the spectrum of representatives on the Panel, one would certainly agree that the collaborations are good; however, there are some prominent hydrogen organizations that are not represented. NASA Stennis and SRNL for example.
- Voluntary participation by DOE-funded organizations appears to be very good, based on the number of safety reviews and safety plans completed.
- It appears that volunteer efforts may be equal to the DOE-funded activity.
- Energy companies, OEMs, and National Labs covered and participating.
- Need to periodically reevaluate the membership of the committee.
- Difficult to assess. Collaboration is actually the organizations that have utilized the service. Over 50 projects have utilized this service.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.8** for proposed future work.

- Continuation and enhancement of existing program.
- Continuation of successful work is going in the right direction.
- The work proposed is consistent with the goals.

Strengths and weaknesses

Strengths
- It is necessary to provide a uniform, multi-disciplined, safety assessment to the DOE research and demonstration efforts.
- Rapid dissemination of safety information.
- Availability of Panel, representing broad expertise.
- Broad spectrum of membership on the Panel across sectors working on hydrogen.
- Experts in the field.
- Strong leadership and approach.

Weaknesses

- There is overlap with other projects. This is not a negative thing, but it exists.
- Maybe missing additional/valuable expertise on the safety of hydrogen.
- Lacking a member on the Panel from one of the energy companies participating in the technology validation program.
- Potential underreporting of real H_2 safety events (who wants to look bad). Need to be aware of this.
- Should rotate membership on the committee for freshness and new/different perspectives.
- Safety questionnaire question is not likely to provide desired results.

Specific recommendations and additions or deletions to the work scope

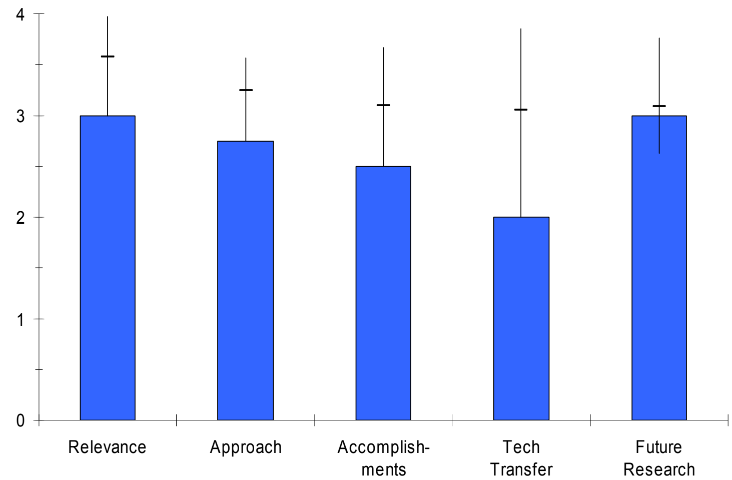
- None.
- Stennis Space Center in Mississippi claims to handle more hydrogen than any other organization in the country.
- Savannah River National Laboratory also makes large claims about working with hydrogen.
- Suggest that both of these organizations be considered for inclusion on the panel.
- Add a member to the Panel from one of the energy companies actually participating in the technology validation program. Actually, this seems to be a glaring hole in the Panel makeup.
- In case it comes up again, I don't recommend adding CNG or LG data to the safety database. The materials are quite different in behavior from hydrogen.
- Consider turning over membership of panel to spread knowledge and broaden experience on the panel.
- Continue the activity as described.

Project # SAP-02: Hydrogen Safety Sensors
Bob Lieberman; Intelligent Optical Systems

Brief Summary of Project

The overall objectives of this project are to reduce or eliminate interferences from humidity and oxygen exhibited by virtually all current optically-based hydrogen detectors and to establish and fully characterize a compact hydrogen detector. Specific objectives in 2006 and 2007 included 1) transfer existing indicator chemistry from commercial to in-house porous glass substrate and improve indicator performance; 2) transfer indicator chemistry from porous glass substrate to polymeric substrate; 3) establish ppm-level response to hydrogen in one or more candidate substrates; 4) establish good hydrogen sensitivity, response time, and sensor performance with little or no response to moisture and oxygen; and 5) develop compact multi-channel detector/test system.

Overall Project Score: 2.7 (2 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.0** for its relevance to DOE objectives.

- Development of hydrogen sensors for a variety of applications supports safety goals of DOE program.
- Low-cost hydrogen sensors are definitely needed for market penetration of hydrogen technologies.

Question 2: Approach to performing the research and development

This project was rated **2.8** on its approach.

- Focused on technical barriers regarding sensitivity, durability.
- Compensation for drift and for moisture might be handled by adding sensors to the same chip, which may be workable, but certainly is not a major breakthrough.
- IOS anticipates that their sensor will be competitive with others, but probably will not sell for significantly less.
- Consideration is being given to add a “scrubber” to eliminate the sensitivity to CO.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.5** based on accomplishments.

- Significant progress toward goals, but several barriers remain in order to reach targets.
- Polymeric substrate longevity is now up to 5 or 6 months, but needs to be 10 to 15 years.
- Dynamic range is only 0 to 10%, but it is possible to duplicate sensor systems and have one operate in the range of 0 to 10% and another in the range of 10 to 100%.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.0** for technology transfer and collaboration.

- Reviewer is not aware of outside collaboration in this effort.
- IOS has had some discussions with potential customers, such as the auto manufacturers.
- IOS is planning to manufacture the sensors themselves or to establish a wholly owned subsidiary; therefore, technology transfer is less critical.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- Plans and target goals are clearly stated.
- Sensors appear to have good commercial possibilities if targets are met.
- There will be need for follow-on funding to complete the development of this sensor; however, I would recommend that it be tied to a solid commercialization plan.
- ISO mentions in one slide the concept of a continuous fiber sensor. This is an excellent idea and should be pursued as a second priority.

Strengths and weaknesses

Strengths
- Project addressing problems in current sensor sensitivity to CO and humidity.
- Working on accurate, low-cost H_2 sensors is definitely a priority.

Weaknesses
- ISO is proposing to correct many of the shortcomings of the sensor by adding a specialty sensor(s) to counteract the response. Although this will work, it increases the potential for sensor failure.

Specific recommendations and additions or deletions to the work scope

- None.
- Add a commercialization plan.
- Initiate the development of the fiber version of the sensor.

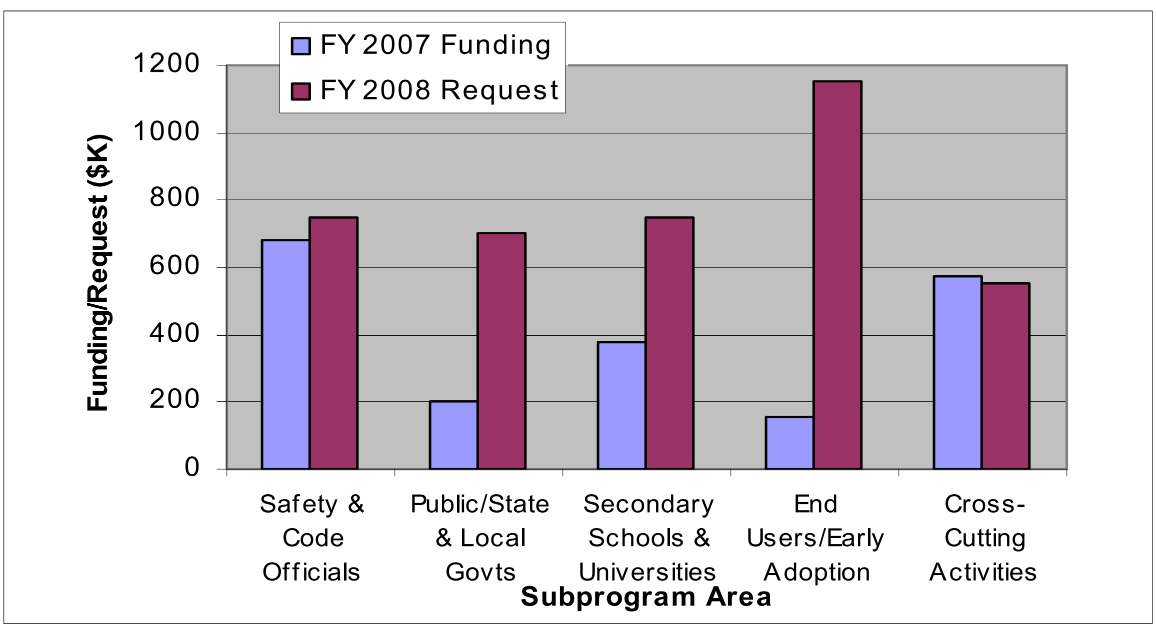
2007
Education
Summary of Annual Merit Review Education Subprogram

Summary of Reviewer Comments on Education Subprogram:

Reviewers continue to express the importance of education, raising awareness of hydrogen and fuel cell technology, and correcting false perceptions or misinformation. Overall, the education subprogram structure and focus were judged to be well-defined and appropriate, with projects well-aligned to DOE targets. Reviewer comments underscored the importance of metrics. Reviewers also noted the daunting challenge of educating a largely uninformed public that is often confronted with mixed messages. Although the FY07 education budget was more robust than in previous years, education projects were recognized for their efforts, flexibility, and success despite limited DOE funding. Reviewers specifically commended the strong partnerships that have allowed PIs to leverage resources and cost-sharing to achieve overall project goals and objectives. They also recognized the benefits of approaches to developing educational materials that involve obtaining input from the hydrogen community and pilot testing with the intended target audience.

Hydrogen Education Funding:

Education subprogram efforts are prioritized to focus on the target audiences involved in the near-term use of hydrogen and fuel cell technology. With funding at the request level, the FY07 budget was the highest it has been in three years; this allowed for support of projects across the education portfolio and the restart of previously-awarded projects that had not been funded since FY04. To support the Hydrogen Program's new market transformation efforts, the education subprogram initiated new activities focused on potential end users and early adopters. These efforts will ramp up in FY08, pending Congressional appropriations. FY08 funds will also support ongoing efforts to educate first responders and code officials, local communities, and teachers and students, as well as new efforts specific to state and local government officials and universities.



Majority of Reviewer Comments and Recommendations:

Reviewer scores for the education projects reviewed were average, with scores of 3.4, 3.3, and 3.1 for the highest, average, and lowest scores, respectively. Scores reflect progress made over the last year. Key comments and recommendations are summarized below. DOE will act on reviewer recommendations as appropriate to the overall scope, direction, and coherency of the education effort.

First responders: This target audience is critical to successful market transformation. Reviewers credited efforts to pilot test, review, and validate the material prior to officially launching it, and noted the pairing of hydrogen and first responder communities as essential to the effort. They also recognized the course usage to date as being successful, but recommended additional outreach and planning to better tie together the introductory course with future work. Certification and the development of regional or re-certification centers were recommended future activities.

Local communities: Reviewers expressed that raising public knowledge above the baseline is a daunting challenge; this effort will help direct people to "the truth" about hydrogen and sort out mixed messages. They also felt that "H2IQ" is a catchy tagline and the sample ads presented were of high quality and maintain the DOE message. They noted that the approach is well defined but flexible and recommended paying careful attention to metrics and collaborating/coordinating this effort with other entities seeking to accomplish the same goals.

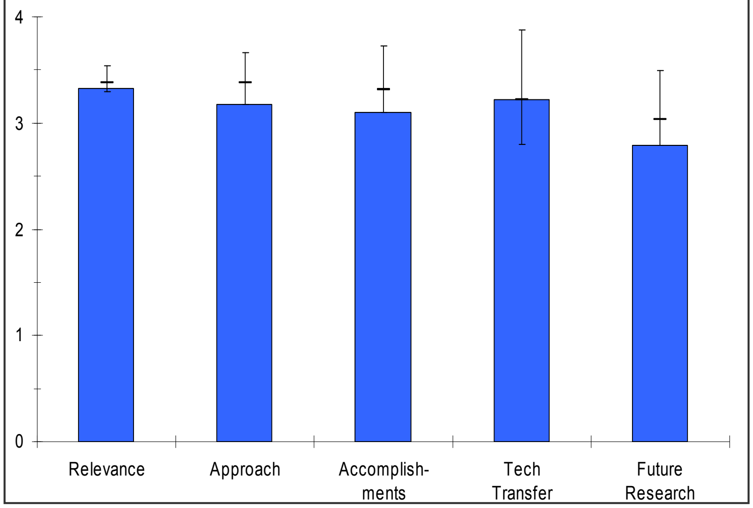
Middle and high schools: Reviewers felt these projects comprise a critical target audience, as students are "technology buyers of the future." They also noted that the projects had been affected by the limited DOE funding, but commended PIs and their teams for building effective partnerships and leveraging resources to survive major budget reductions and achieve success. In general, reviewers felt that the approaches taken to materials development were effective and suggested that projects pursue an aggressive dissemination strategy to maximize the usage.

Project # ED-01: Hydrogen Technology and Energy Curriculum (HyTEC)
Jim Zoellick; Schatz Energy Research Center

Brief Summary of Project

The purpose of the HyTEC program is to educate high school students and their teachers about hydrogen fuel cells. The objectives of the program are to 1) develop, test and disseminate three curriculum modules and integrate hydrogen into existing Lawrence Hall of Science high school materials; 2) develop and implement a professional development plan for teachers who will use the materials; 3) develop a model for collaboration among school districts, scientists, transportation agencies and other leaders in the field; 4) disseminate the materials to a broad national audience; and 5) evaluate the quality and effectiveness of the curriculum materials and professional development strategies.

Overall Project Score: 3.1 (4 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

- Addresses key target audiences through program.
- It would be a great asset to expand to other categories besides Bay Area – other consortiums or groups could implement some approach / strategy.
- Project is relevant to the program – high school student and teacher education.
- Educating high-school students is important to make them comfortable with hydrogen technology: "children are our future," as others have said.
- Fits with targets for DOE program to improve knowledge for the next generation of technology users.
- Scaled-back objectives are appropriate for funding level but still provide benefit for the hydrogen education program.
- One of the four target audiences for education is students – this project covers high school chemistry and environmental science classes.
- The issue-based approach improves the relevance of the modules – why is a shift being made to hydrogen?

Question 2: Approach to performing the research and development

This project was rated **3.2** on its approach.

- Partnered with organizations that help achieve objectives.
- Modified program due to lack of funding – still addressed key points (standards).
- Completed a significant number of tasks with limited funding from DOE.
- Curriculum tests with varied and diverse group of students are very important.
- Project partners represent complementary capabilities and resources to accomplish the project objectives.
- The original project approach appeared to be well defined but the approach does not appear to have been re-scoped. This project was obviously greatly impacted by the availability of funding.
- High school students are a critical audience; they will be the technology buyers of the future.
- Wide-ranging overview of topics for the curriculum; this ensures good coverage for educating the audience and fits with standard high school chemistry topics.

- Good hands-on activities: the heat energy of fuels is an interesting addition that will probably serve these students when they hear about all alternative fuels, not just hydrogen. CO_2 calculations are good additions too; they get students thinking about impact of fuels on climate change.
- Issue-oriented science makes information relevant; not just theory that high school students may not think is valuable.
- Having a replacement for existing science curriculum ensuring core subjects are covered is key to fitting into a very crowded field of science topics.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.1** based on accomplishments.

- Developed very relevant and important curriculum activities.
- Hands-on approach is very important – kids respond much more when they are involved.
- Stack in a box – key tool for program – shows fuel cell potential.
- Video segment – great way to reach young audience.
- While it is not clear what phase I objectives were, the curriculum modules developed appear to be extensive and rigorously tested and reviewed.
- Accomplishments are extensive, especially given the funding issues.
- Modules developed appear interesting and practical for students.
- Hands-on lab activities are important.
- Physical "puzzle" model of redox is interesting approach for what can be a difficult-to-understand chemical theory.
- Good linkage of lab-scale fuel cells (single cell) up to full-scale fuel cells for improved understanding.
- We are looking forward to a final chemistry module on the market with kit. Wish it was further along.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.2** for technology transfer and collaboration.

- Contractor is contributing a significant portion of funding to keep program going.
- Great outreach with AC transit.
- Classroom curriculum trials at 3 high schools is a good start with defined metrics, i.e. 3 high schools ~300 students.
- Curriculum trials are based in California. Future work might include a more national scope.
- Very effective partnership between the curriculum testing and AC Transit "real world" applications of hydrogen and fuel cells.
- Having a real-world operator of fuel cell technology (AC Transit) as partner is a good addition; should bring a practical focus to the educational materials.
- Professional videographer is a good addition as well.
- Good to have a partner (Lab-Aids) with a focus on widespread distribution of materials.
- Good approach to team effort and roles – a complete path to market.
- Science teacher outreach via SEPUP system is a strong conduit to use.
- Obtaining matching funds was a major help to keep project moving.
- Science teacher conference presentations are a good outreach tool.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.8** for proposed future work.

- Program expansion likely.
- Making videos and curriculum available to others would be extremely useful – online would make it cheap to do.

- Project next steps are not clear – status was focused on lack of funding. Perhaps this is being addressed as funding becomes available.
- Field testing outside California is good; should provide an interesting contrast to the fuel-cell friendly California environment.
- Ambitious future research plan; funding will hopefully fit the ambitions.
- Timelines for completion of module and kit are needed.

Strengths and weaknesses

Strengths
- Key partners.
- Accomplished a lot with little money.
- Video teaser is a very effective communication tool.
- Issue-oriented approach gives practical experience (vs. dry and "uninteresting" theory).
- Hands-on focus with practical applications is good.
- Testing with variety of student groups – makes it more applicable for audiences the curriculum will reach.
- This project survived with a two year break in funding – kudos.
- It also weathered a major budget reduction – again kudos.

Weaknesses
- Limited range (Bay Area).
- Although the project has been significantly underfunded they have moved forward with their project partners in some areas – there didn't seem to be a defined completion for the curriculum development.
- Funding issues have limited the reach of this program.
- The pathway to completion needs to be strengthened.

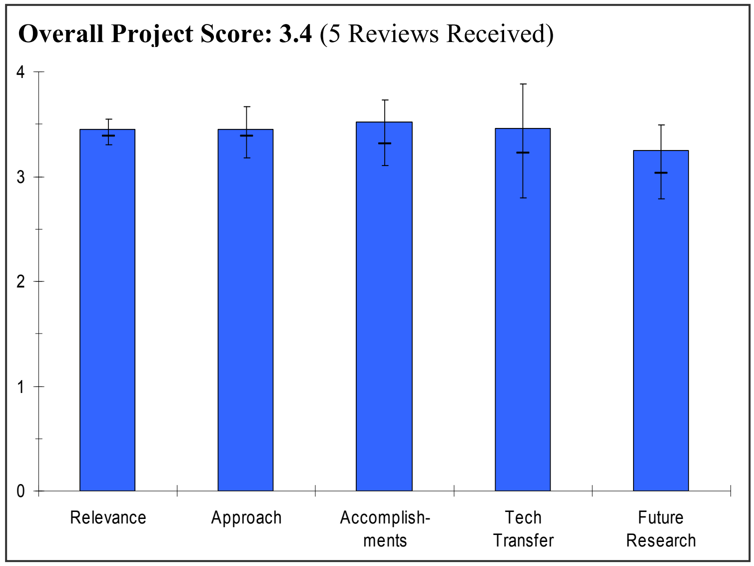
Specific recommendations and additions or deletions to the work scope

- Project scope needs to be redefined with a phased approach with DOE and project partners so the project can demonstrate accomplishments as funding is available.
- Video teaser should be shared with other DOE-sponsored education activities.
- Nothing specific.
- None.

Project # ED-02: H2 Educate!
Rebecca Lamb; NEED

Brief Summary of Project

The overall objective of H2 Educate is to develop, design, and deliver a first-class comprehensive middle school hydrogen education program including: training, classroom materials, technical and best-practices exchange, and evaluation. The objectives for fiscal year 2007 are to 1) deploy materials via teacher training and professional development opportunities; 2) provide technical support for schools that previously entered the program, and collect data for revisions; and 3) work to expand the reach of the program with new partners able to support training workshops at the local level.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

- Middle school students and teachers are a key audience.
- Able to expand in NY to also reach general public.
- Relevant to the MS target audience as identified by the program.
- Project goes beyond the DOE program objectives to address teacher/education requirements and standards ensuring the interest in and use of the curriculum.
- Middle school education project will fit well with the associated high school project; these should be complementary activities.
- Well-linked to the need to address information and education barriers.
- This project fits the student target audience – middle schools.

Question 2: Approach to performing the research and development

This project was rated **3.5** on its approach.

- Partnered with numerous organizations to complete goals.
- Utilized existing network of NEED teachers to accomplish goals.
- The defined curriculum is national in scope accomplishing both the DOE objectives as well as addressing value to the teacher audience.
- Wise approach to "ask before doing" to understand needs of the target audience and users.
- Focus on deployment of the curriculum to actual users is useful; materials do not teach anyone if they don't reach anyone.
- Good mix of states that have active interest in hydrogen programs and states that don't have as much interest.
- Good idea to have modular and flexible approach to fit within time available in the classroom.
- Impacts due to funding.
- Kits should be standardized between all the different funded activities so one agency or organization can get quantity discounts.
- Advisory board used.
- Pilots, workshops, and feedback.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.5** based on accomplishments.

- Ensured program complied with national standards.
- Expand project in NY to reach general public.
- NEED has done an exceptional job responding to the funding impacts, the scope of work was revised and creative options were obviously pursued to accomplish both the curriculum development and deployment.
- Deployment activities appear to have been effective (good to have it online).
- Online print availability of materials provides flexibility to meet teacher needs.
- Development of these materials in less than the time estimated is quite an achievement.
- The "demonstration car" will keep interest up with the students.
- NEED initiative to find local funding for maintaining deployment efforts when DOE funding was not available is important.
- Impacts due to funding.
- Not much impact this year with DOE funding, more with state or local funds.
- Project is in final dissemination stage.
- Curriculum finished early.
- Good connection with EIA kids page.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.5** for technology transfer and collaboration.

- Diverse group of funders and contributors.
- NEED's access to teachers makes project successful.
- Partnering with groups that will help expand and sustain program.
- Important metrics defined and measured – reach teachers and students on a national level.
- Excellent metric – over 4000 teachers.
- Project goes beyond MS teachers and students to general public, even EIA.
- Very effective deployment strategy.
- Curriculum design is extremely flexible for teachers.
- Good list of partners (NHA, NYSERDA, PG&E, BP).
- Working with EIA to demonstrate hydrogen to analysts is an interesting side project to increase their [analysts] practical understanding of hydrogen.
- Variety of workshops to present the program to teachers are important.
- Good, more DOT involvement would be helpful.
- Targeted workshops used.
- 4,000 teachers reached.
- Website downloads used.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.3** for proposed future work.

- Expanding in VA, adding markets and module will ensure continued success.
- Continued deployment strategy has excellent promise both to the MS as well as general public.
- Maintaining up-to-date information is critical, especially for a fast-changing field such as hydrogen. Annual updates are a good idea.
- Would have liked more information on future research. (This may be a function of the lack of funding).
- Need more aggressive strategy to expand the materials and link to all the projects.
- Further outreach workshops needed.
- Project moving to completion.

EDUCATION

Strengths and weaknesses

Strengths

- Able to achieve goals with limited funding.
- High demand.
- Educating more than students and teachers.
- Project is very well defined; curriculum was developed with a defined national scope of implementation goal.
- This project is a fantastic investment by the DOE Hydrogen Education Program.
- Modular curriculum allowing teacher flexibility in amount of time needed.
- Collaboration and cooperation among several states, including key "fuel cell states" like California.
- Good initial effort.
- Good products.
- This project survived with two years of no funding – kudos.
- Obtaining matching funds to dissemination materials and kit information has helped.
- Flexible training times used.

Weaknesses

- No weaknesses are evident – except for the funding component but it was addressed and overcome by the project team.
- Lack of funding limited some of the reach of the program.
- Cost of the materials can be an issue for teachers.
- Project modules are expensive due to toys.
- More linkage of all the funded projects to limit FC modules, toy vehicles or electrolysis to a single design or manufacturer to get large buy reductions in cost.
- Kit is $500 which may be beyond reach of some teachers.

Specific recommendations and additions or deletions to the work scope

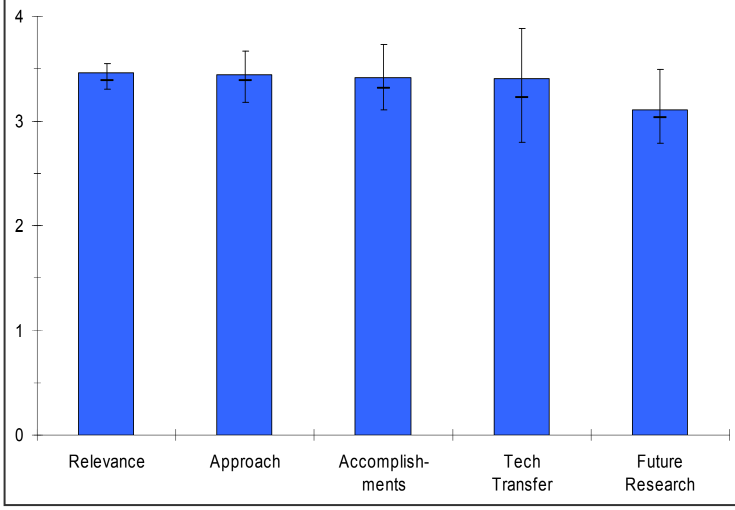
- None specific.
- Fully fund project and conduct more state education activities.
- None.

Project # ED-03: First Responder Education
Marylynn Placet; PNNL

Brief Summary of Project

The long-term objective of this project is to support the successful implementation of hydrogen and fuel cell demonstration projects and market transformation by providing technically-accurate and objective information about hydrogen to first responders. The focus is on first responders such as fire, law enforcement, and emergency medical personnel who must know how to handle potential incidents. The objective for fiscal year 2007 is to develop and disseminate education materials that pertain to hydrogen safety, aimed at the first-responder audience.

Overall Project Score: 3.4 (5 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

- Well-reasoned approach to education for emergency professionals.
- Long overdue effort within the program, progressing at an excellent pace.
- First responder education is important to successful technology deployment; education gaps for this group have caused issues with other technologies (e.g., hybrid vehicles, natural gas vehicles).
- Critical to get first responder buy-in for technology projects; this education will help greatly.
- Critical need to develop training materials for first responders.
- Linked to safety codes and standards.
- This training hit a key target audience need.
- It will also help with permitting by fire departments – this gives a double impact.
- First responder education is critical to the success of hydrogen market transformation.
- Feedback from users of Task 1 awareness course (and number of users) indicates that the activity is very relevant to first responders.
- The PI did not address specifically the tie-in between the goals of the Hydrogen program and the work done under this activity.

Question 2: Approach to performing the research and development

This project was rated **3.4** on its approach.

- Appropriate technical level for this specific audience.
- Easy-to-use web-based format, with additional formats also made available.
- Well-tested prior to launch, thus ensuring accuracy of information and understandability.
- Project appears to address major barriers outlined.
- Web-based tools are an excellent way to distribute information widely.
- Focus on basic information is appropriate; want to avoid assuming people know things they don't necessarily know.
- Pilot testing to refine curriculum with HAMMER is useful: improves final product.
- Project has addressed both the curriculum and the distribution of the course to the audience.
- Good approach.
- Process for workshops to develop and validate materials was good.

- Certification process requires more focus.
- The web based training with CDs for train the trainer has worked very well.
- Very strong ties to the first responder community through HAMMER. This was a major key to success.
- This project built on strong prior work (pilots with comments and feedback).
- Performer has completed 1 of 3 Tasks (Awareness-Level Course Development); other two Tasks are 60% and 5% complete at this time.
- Review of pilot awareness course was completed very comprehensively, ensuring high accuracy.
- Unclear how the course could be made mandatory (through State regulations, etc.) to increase the number of first responders who are trained by web.
- Task 2 Outreach approach is satisfactory to achieve a large number of users.
- Task 2 seems to target a number of vehicles for awareness (conferences, etc) without PI explaining why those vehicles were chosen.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.4** based on accomplishments.

- Good progress, especially considering relatively low funding.
- Development of props will require increased funding, which should be provided.
- Awareness-level online course appears clean, concise, and well-done. It delivers short educational messages, and avoids clutter and confusion.
- Combination of static slide text and video in web-based course is a good idea to maintain viewer interest and show real-world activities (such as vehicle refueling).
- What is done with quiz results from online courses? They probably show the effectiveness (or lack of effectiveness) of the online course for a given audience quite well.
- Good use of up-to-date Web tools (particularly Flash animation), which provide more interesting visuals.
- Excellent response on course.
- Need more products for reinforcing info.
- This project has come a long way since last year.
- 240 people taking course weekly online is fantastic outreach achievement.
- PI did not present any performance indicators (effectiveness in particular) that are measurable, aside from number of users of awareness course, which does not explicitly link to improved first responder actions.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.4** for technology transfer and collaboration.

- Good integration with HAMMER facility.
- Excellent use of Hydrogen Safety Panel expertise, and the expertise of the hydrogen community.
- Good distribution effort to the target audiences.
- HAMMER collaboration is useful and provides credible link for this project to the first-responder community. Good use of a local resource.
- Wide-ranging review process for online course with major stakeholders is a plus. Careful addressing of comments shows in the final product.
- Good coordination across program and agencies.
- Very strong outreach ties to first responders – broad multi-state.
- Good partnership with the HAMMER Institute, which possesses the skills needed to complement PNNL.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.1** for proposed future work.

- Props will be a great addition to first responder training.

- Hands-on prop-based course should be effective for this practical, pragmatic audience. Hope sufficient funding will be available from various sources to develop high-quality props, as this will enhance project credibility with the audience.
- Conference and magazine article outreach should continue.
- Need more validation.
- Complete FC vehicle and implement its use.
- Prop-based mobile training fills the needed hands-on requirement for fire departments.
- Further outreach is essential.
- The CDs help "train the trainers."
- Continuous improvement for Task 1 awareness course is valuable effort.
- PI did not present an actual plan that includes future events that would show the rationale for choosing future events, such as prop-based work.

Strengths and weaknesses

Strengths
- Materials are being developed at the appropriate level for the target audience.
- Large community of experts is being called upon to review materials, ensuring accuracy and understandability.
- Ability to interact on web course with the users through comments page is a plus.
- Well-done Web visuals.
- Good targeting of an important audience.
- Range of information, from basic hydrogen information through to more complex information (hydrogen vehicle refueling, etc.).
- Summary poster for first responder facilities.
- Good team.
- Well linked to application.
- Experienced in critical training.
- Superb work!
- This project pre-positions HFCITP for early markets and permitting efforts.
- Good statement of barriers that are addressed through this activity.

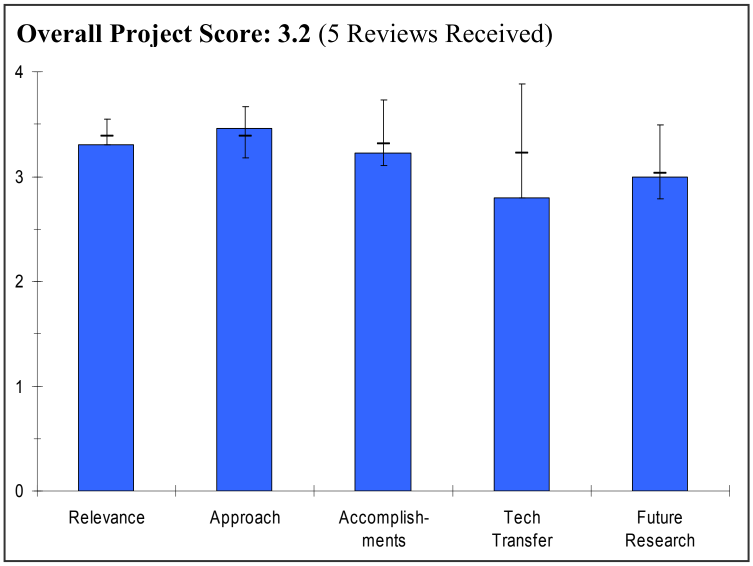
Weaknesses
- Funding needs to be higher and sustained for the prop development and use phase.
- Nothing specific.
- Need to focus on certification.
- Develop regional training or re-cert centers.
- Wallet card on key facts.
- PI did not present an actual plan showing the criteria for how Tasks are selected or how future Tasks will be tied into the project.

Specific recommendations and additions or deletions to the work scope

- Some of the modules might be interesting for audiences beyond first responders: how might DOE get other users to take advantage of these well-designed modules. How can this complement the other education programs?
- Add the "certification tools" that were discussed (if funding available).
- Fully fund.
- Complete more modules.
- None.

Project # ED-04: Increasing "H2IQ": A Public Information Program
Henry Gentenaar; The Media Network

Brief Summary of Project



The objectives of this project are to:
- Transmit our message via the communications channels that audiences use;
- Develop and disseminate resonant messaging that communicates to the general public basic facts about –
  - Hydrogen as a fuel/form of energy
  - Fuel cells as an alternative to traditional power technologies
  - The DOE Hydrogen Program;
- Generate interest and increase public requests for more information;
- Give the Hydrogen Program a communications mechanism with a flexible framework for reasons of timing and budget;
- Support the DOE brand;
- Help position the Program in the mind of the public;
- Build recognition of hydrogen and fuel cell technologies;
- Make the most of DOE resources and provide a gauge of success.

These objectives are planned to be accomplished using print, radio, television, satellite, and new forms of media. The project will coordinate closely with the Technology Validation Sub-Program and focus initially on Hydrogen Learning Demonstration project areas/locations. The primary target audience is the general public.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

- General public is a key audience that needs to learn more about hydrogen.
- Public can influence law makers, media, companies in area to move toward hydrogen.
- Project has direct relevance to the general public audience.
- Reaching the general public with up-to-date, non-biased information on hydrogen is critical to meeting the ultimate goal to deploy hydrogen technology; if the general public isn't comfortable, they won't adopt the technologies.
- Important to sort out mixed messages to provide the "truth" about hydrogen.
- The general public is as broad a target audience as you can get. It is a daunting challenge to raise the baseline knowledge, but one has to start somewhere. A solid beginning.
- PI is raising awareness by introducing hydrogen to the general public, a clear component of the hydrogen program.
- PI did not clearly link the project's efforts to the hydrogen plan.

Question 2: Approach to performing the research and development

This project was rated **3.5** on its approach.

- Not sure if radio is most effective way to go – a lot of people have satellite radio or listen to own source of music while in car (CDs, iPods).
- How do you know this specific program is leading to increase in knowledge when there are so many other conduits of fuel cell information and hydrogen resources (NHA, USFCC)?

- The project approach is well defined and addresses a broad scope of communication methods.
- Project products can be applied to every target audience defined by the program.
- Excellent understanding of the audience, technologies, and messages.
- "Positive message" is important, and DOE needs to do more of this (vs. negative "energy hog").
- Delivery of basic hydrogen information to a tech-savvy market through unconventional media outlets is a good approach; the audience most familiar with these vidcast/podcast technologies also likely to be interested in (and to purchase) hydrogen fuel cell technology.
- H2IQ is a catchy tag line.
- Flexible structure for the media tactics.
- Addresses fragmented nature of traditional media (especially television).
- Coordination with locations where hydrogen validation projects are underway: targets the message.
- Addressing quick targeted messages is a key and strategic approach.
- Non-traditional media approaches being used.
- Tied to tech validation and market transformation.
- The Communications Blueprint is very important to structure the range of the task. The homework was essential.
- Solid identification of barriers.
- Performer's phased plan for messaging allows good flexibility, which is important given the complexity of the hydrogen subject.
- PI demonstrated sophisticated understanding of the subject matter and how it applies to hydrogen.
- Clearly stated target audience for the performer's work and how to reach them.
- Strategic approach is well-defined and explained.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.2** based on accomplishments.

- Budget was out; tailored the project to focus on less expensive ways to distribute the message.
- Products developed – radio and podcast strategy promises to be very successful.
- Defined message and understanding the method of communication is well done.
- Clear blueprint of "what do people think now" and how can we facilitate change?
- Clear, concise messages (hydrogen is safe, meets energy independence and cleaner environment needs).
- Good mix of audio and video deliverables, good use of web as a wide-ranging broadcast medium.
- Maintains the DOE message (energy independence, environment) among the radio and podcast materials.
- Sample ads were high quality.
- Steady progress made.
- Wish we were further along.
- "Communications Blueprint" is confusing – unclear what the slide is trying to convey since it is mixing both target objectives with deliverables and other information.
- PI presents the ability to successfully carry out the planned work.
- PI did not present clear indicators or other ways of measuring success (or effectiveness, efficiency, cost or benefits), except for brief mention of number of log-ins to the H2IQ website.
- Performer has made progress in navigating the DOE bureaucracy in getting radio spots and podcasts/vidcasts approved.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.8** for technology transfer and collaboration.

- Program partnering with iTunes – key to distribute to large audience.
- Collaborating with states with demonstrations – need to make sure everyone has access.
- Products developed – radio and podcast deployment strategy promises to be very successful.
- Expanded use of these products hold great promise if they can be used throughout hydrogen outreach community.

- It is early in the project but the strategy of deployment is planned and metrics will be available next year. (It is too early to evaluate deployment success.)
- Not much collaboration now, not much detail on potential collaborators. Hope more detail will be available at next meeting to better gauge collaboration.
- Will auto manufacturers/energy companies be approached as collaborators?
- How about major media networks, AOL, etc.?
- Good to involve EERE OTAO as a planning partner.
- We are looking forward to roll out of podcasts and vidcasts.
- No information presented about collaboration in presentation.
- Coordination with states, as mentioned during the discussion period, will be very important to try to leverage state and city resources, both financial and institutional (existing communication channels) but currently does not exist.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- Deepening markets is key to reach audience.
- Metrics are defined and the future plans are designed to respond to successes and changing opportunities.
- Future plans seem appropriate.
- Measurement of success is critical to quantify success of message delivery (iTunes statistics, web traffic hits/time spent).
- This is an important fit to early markets.
- PI did not present any substantive information about future activities except continuing existing activities.

Strengths and weaknesses

Strengths
- Radio spots are clear.
- Focusing on areas with demonstrations.
- Excellent defined scope – defined to be flexible and responsive to both priorities and leverage funding.
- Great understanding of different communication technologies.
- Excellent project and a great value.
- Looking at new media outlets for the message (vs. standard website/print ads/etc.).
- Flexible campaign to fit local needs and budgets.
- Effective concise message fitting DOE needs (energy independence).
- Focused, targeted campaign that doesn't waste time on areas without hydrogen activity.
- The Communications Blueprint provides key structure to this effort.
- Documenting downloads will be an important metric.
- Performer had significant familiarity with the various communications methods and how to provide outreach to the general public.

Weaknesses
- How do you tell if it is working?
- How do you ensure people will hear message?
- At present, lack of visible collaboration could be a weakness, but this appears to be a topic to address in FY07.
- As with other education projects, budget appears to limit progress to some extent.
- Unclear how this activity will progress without a proposed plan that includes, for instance, the sequential introduction of radio spots into specified markets for XX reasons.

Specific recommendations and additions or deletions to the work scope

- Formalize the processes to distribute podcasts and vidcasts to interested stakeholders.
- None.

2007
Systems Analysis
Summary of Annual Merit Review Systems Analysis Subprogram

Summary of Reviewer Comments on Systems Analysis Subprogram:

The reviewers considered the Systems Analysis Subprogram essential component to the Hydrogen Program mission and critical to the President's Hydrogen Fuel Initiative and AEI. The projects are considered appropriately diverse and focused on addressing technical barriers and meeting targets.

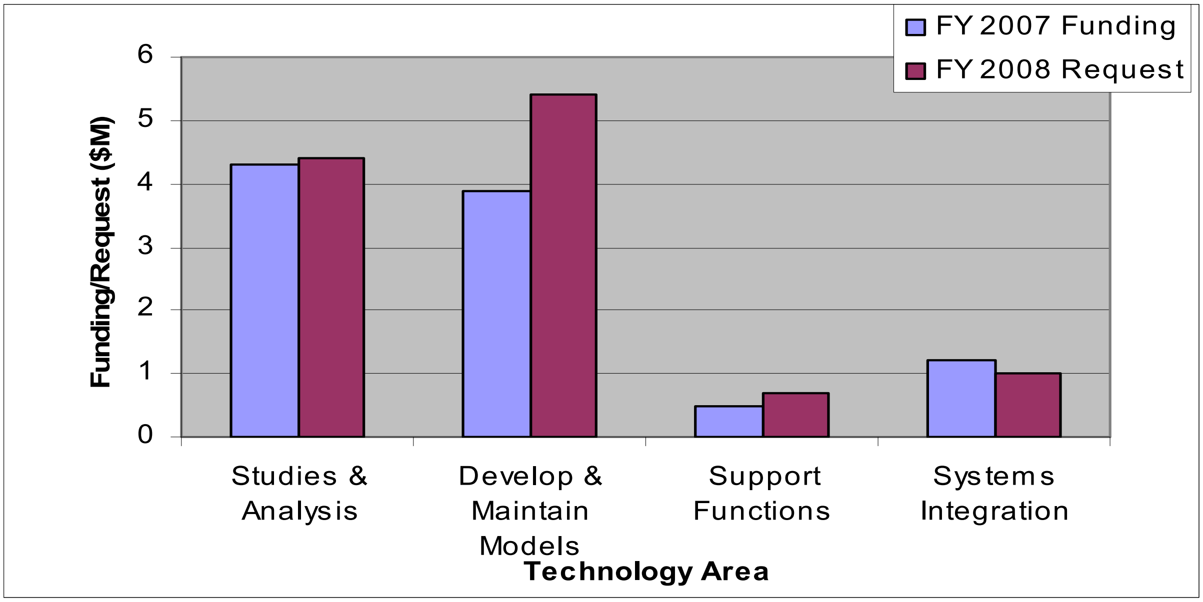
In general, the reviewers noted that Systems Analysis is a complex subprogram but is receiving the appropriate management attention. Some reviewers commented that the subprogram is well managed and has adopted an organized approach for analytical support of the Hydrogen Program, which is consistent with addressing the comprehensive list of identified barriers.

The major concerns identified by the reviewers for Systems Analysis were: 1) safety variables should be considered in systems analysis and consumer choice modeling; 2) fuel purity and the impact on performance and cost tradeoff analysis should continue; and 3) model validation and peer review is critical for sound and creditable analysis. The Systems Analysis subprogram will continue to address these issues and will be incorporated in the Systems Analysis Plan..

Finally, the reviewers commented the analysis and model portfolio was complete and covered the analysis topic. They indicated the analysis Multi-Year Research, Development and Demonstration Plan (MYPP) barriers were being covered and put into the proper perspective.

Systems Analysis Funding:

The funding portfolio for Systems Analysis primarily addresses the model development and required analysis to support the Technology Readiness Goal. The requested 2007 funding profile, subject to Congressional appropriation, addresses the National Academies' Report recommendations and provides greater emphasis on transition, resource, and infrastructure analysis.



Majority of Reviewer Comments and Recommendations:

In general, the maximum, minimum and average scores of the reviewers of the Systems Analysis projects were 3.5, 2.4 and 3.1, respectively. The Systems Analysis project portfolio includes a mix to address the "analysis and modeling gaps" of the subprogram and the transition requirements. The major recommendations for the Systems Analysis projects are summarized below. DOE will act on the reviewer recommendations for the overall Systems Analysis effort.

- **Impact of Hydrogen Production on U.S. Energy Markets Project:** Focus on the linkage and integration with other models to insure consistent inputs and assumptions are being used. Need to include the impact of highly visible government programs and policies.

- **Analysis of the Hydrogen Production and Delivery Infrastructure as a Complex Adaptive Model Project:** Ensure the agents representing industry include risk profiles, spending practices and business goals to maximize profit within companies which can increase or decrease adoption rate. Need to develop a validation method for the model.

- **HyDRA-Resource Analysis:** Ensure this model is beta tested and aligned with business/industry decision makers. Need to add sites for geologic storage of hydrogen.

- **Macro-System Model Project:** Ensure common and consistent assumptions and inputs are utilized in the linked models. Need to add hydrogen quality/cost tradeoff and stochastic modeling in the model.

- **Hydrogen Quality Analysis: Production to Fuel Cell:** Ensure the model is peer reviewed. Focus on fuel cell performance in the model. Need more collaboration outside the tech team.

- **Hydrogen Transition Modeling and Analysis: HyTrans v.1.2:** Ensure the model is validated and peer reviewed. Focus future studies with the model on sensitivity analysis.

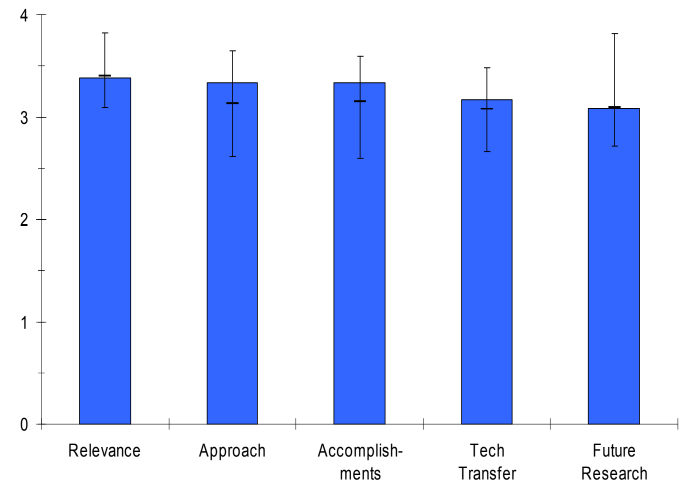
- **Well to Wheels Analysis of Hydrogen Pathways with the GREET model:** Need to add plugins representation in the model. Need to obtain feedback from users and interface with stakeholders.

Project # AN-01: Hydrogen Production Infrastructure Options Analysis
Brian D. James; Directed Techs.

Brief Summary of Project

The objectives of this project are to 1) create an analytical tool robust enough to assess the impact of different assumptions on hydrogen infrastructure development; 2) exercise the tool to determine the key drivers of the hydrogen transition; and 3) suggest to DOE areas of further research based on the most influential parameters in the infrastructure development. The unique features of HyPro include its ability to evaluate infrastructures with varying utilization over lifetime; its ease of use; an interface aimed for use by a wide audience; a structure that can be incorporated into the Macro Model; the allowance for investor demand foresight; incorporation of stranded asset logic; user input of yearly varying hydrogen demand, unit efficiencies, and capital costs.

Overall Project Score: 3.3 (6 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.4** for its relevance to DOE objectives.

- Model designed to analyze the transition to H_2 infrastructure.
- Supports objectives of H_2 production and delivery cost.
- The model is useful for calculating the capital and operating costs of a hydrogen infrastructure and the resulting hydrogen fuel costs.
- The model is useful for evaluating sensitivities to differing assumptions and scenarios.
- I like the incorporation of NPV calculations to the techno-economic models previously used.
- This is an important project that will help DOE understand the key drivers of a hydrogen transition.
- This project is one of several that are addressing the issue of transition to hydrogen-based transportation vehicles and infrastructure.
- It is not clear how the results of this analysis will be used and by whom.

Question 2: Approach to performing the research and development

This project was rated **3.3** on its approach.

- Approach assumes a H_2 demand as a yearly input.
- Based on demand, model grows infrastructure by building H_2 production and delivery capacity.
- The objective function to minimize cost is a good approach.
- Uncertainties in technology development and capital cost reduction appear to be well captured via use of sensitivity analysis (optimistic vs. pessimistic brackets).
- While the results are very well documented and understood, the project is based on perfect foresight of demand which in a real world is unrealistic. The PI could evaluate the use of a probabilistic approach (via Monte Carlo simulation) in order to simulate demand and examine the impact on the results.
- The modeling approach to production options and costs is sound, given a somewhat simplistic user-defined demand. The model incorporates all realistic production pathways.

- The basic structure is there, and the incorporation of NPV calculations is very nice. As a potential future user I would like to see more validation, and more collaboration with existing OEMs especially in the area of forecourt reforming. I caution you to not rely on new vendors like H2Gen for FC CAPEX reductions over time.
- Might want to consider a more detailed understanding of tradeoffs between potential scale of a technology, building multiple units to reach capacity, etc. This would add robustness to the model results and would help give the model more credibility.
- Model development in MATLAB is a good approach.
- Although better than last year, still too much input from distributed hydrogen production developers, especially SR.
- Lowest cost options won't/can't always be selected. In reality a mix of production/dispensing options will be developed.
- The project is using an Excel-based database (from H2A) and MatLab algorithms, where the user enters the annual hydrogen demand.
- The model then selects the least-cost production pathway.
- The model incorporates many different production (both central and forecourt, including nuclear hydrogen and hydrogen from coal) and delivery pathways.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.3** based on accomplishments.

- Project is on schedule & producing predictions of H_2 cost from various production and delivery options
- The model projections to date are limited by the input assumptions, and produce fairly obvious (in hindsight) results.
- I think the valuable contribution of this project will be the development of the approach, which should pay-off if it can be incorporated into the MSM.
- Economic analysis (such as costs) have been well revised since 2006 in order to capture the wide range of distributed SMR costs and the PI appears to be interacting very well with the relevant industry partners in obtaining costs. Therefore, he is well placed to reach consensus with industry on economic analysis.
- Good enhancements to the model were added during the past year.
- The model was exercised, and sensitivities were analyzed. The net result was that some key drivers were identified.
- New HyPro is much more useful than H2 Sim 1.0.
- HyPro still hasn't been used to evaluate some key drivers/barriers (e.g., >> 40 stations initially required)
- Many assumptions appear to be too optimistic (e.g., number, utilization, and cost of forecourt stations; carbon sequestration costs; cost/size of pipelines; redundant components in the early years).
- Although given a very difficult task, HyPro model doesn't appear to be very easy to use and may be too complex for error-free, transparent results.
- Analyzed the Los Angeles basin as a base case.
- It is interesting that for many of the cases shown, the cost of hydrogen is essentially flat from 2020 to out-years.
- The cost difference with or without carbon capture and sequestration is very small.
- Even with a renewable mandate, ethanol only plays an interim role at low demand levels.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.2** for technology transfer and collaboration.

- Good collaborations with university (UC Davis) and some industrial partners.
- The project appears to be very well connected with the H2A, UCDavis, HDSAM and HyTrans. The PI could consider interfacing with an agent-based modeling approach (such as the work done by RCF), which could impact the demand scenario based on actions taken by investors (on whether or not production capacity will be expanded or added).
- Collaboration with industry is evident. Information flow seems to be mostly in the form of input from industry; not clear to what extent the model and model results are being used by others, or for others.

- Not well-coordinated with the latest H2A model development work.
- Doesn't appear to be thoroughly vetted by industry, especially auto OEMs.
- The project has several companies on the advisory board.
- It is not clear how actively involved the advisory board is in the conduct of the project.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.1** for proposed future work.

- Project is nearing completion.
- Future plans for the model need to focus on how it can be coupled to the Macro-system model in a way that eliminates the requirement to assume a H_2 demand in time.
- Plans for the next stage are clear and consistent.
- Planned updating of databases with latest H2A and HDSAM values is essential.
- Further sensitivity analyses are likely to be more useful, than simply running the model for additional cities, in terms of identifying incentives required or areas for further DOE research.
- National trends should also be included in the scope of work.
- Update data and parameters in/from contributing models, such as HDSAM.
- Examine other scenarios, regions (New York?).
- Identify needed incentives and research areas for DOE to consider.
- The "value" of the identified future work was not clear.

Strengths and weaknesses

Strengths
- The computation algorithm to choose production technology for build-out to meet demand should be useful to the MSM effort.
- I like the build-out approach, but the results to date seem a bit obvious in hindsight; I think the approach will prove it's usefulness if it can be combined into the MSM.
- Project objectives are clearly stated and well defined.
- Industry input is a strength of the project.
- NPV capability.
- Despite the enormous amount of information to cover, the presentation was clearly presented.
- The model includes a fairly comprehensive set of hydrogen production pathways.

Weaknesses
- The need to input a demand curve in time is the main limitation.
- This project does not include investor risk profile/behavior and decision behavior in order to make key business decisions to install capacity.
- Competitive analysis among distributed SMR investors is also not included in the analysis.
- Need to increase the amortization time allowed for pipelines to more than the 20 years currently in the model.
- Would work on obtaining more realistic Capital Expenditure estimates.
- The model has not been used to understand key drivers and, more importantly, potential technical/cost barriers to a hydrogen transition (i.e., some assumptions are too optimistic).
- Need to show examples of effective use of results from the model.
- The degree of confidence in some data (production pathways) is greater than in others, e.g., steam-methane reforming versus nuclear hydrogen. This needs to be clearly accounted for, even if the data come from other models, such as H2A.

Specific recommendations and additions or deletions to the work scope

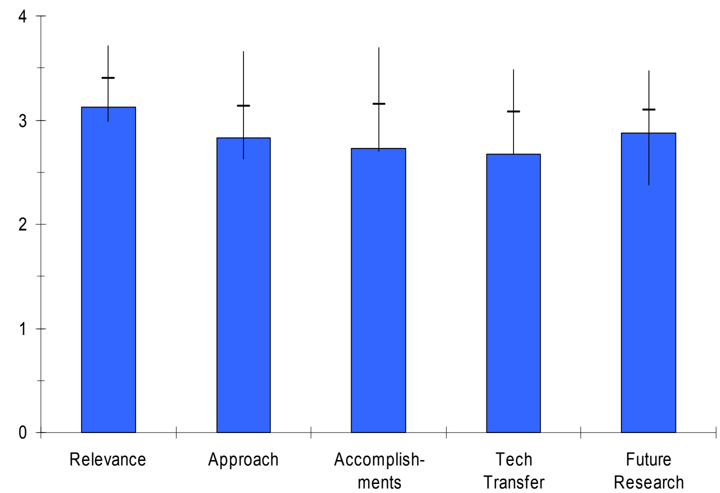
- The fixed demand curve limitation is not a problem if the model can be incorporated into the MSM in a way that the demand is determined by another model.

- User control (possibly through integration with MSM) of the pathway definitions would be useful; for example, different lifetimes for pipelines or other technologies.
- The project would benefit more if investor analysis and/or risk analysis studies are integrated into the decision-making process on whether or not to build capacity every year.
- Hydrogen fuel purity requirements could alter the relative costs of hydrogen from the different pathway options, and adding this should be considered.
- While the model does calculate stranded assets, no quantitative results were presented to indicate how significant an issue this may or may not be, or what policies, if any, should be considered to ameliorate the effects.
- Project needs closer coordination with hydrogen delivery analysis teams and thorough vetting by industry (especially auto OEMs and energy companies).

Project # AN-02: Impact of Hydrogen Production on U.S. Energy Markets
Harry Vidas; EEA

Brief Summary of Project

Overall Project Score: 2.8 (7 Reviews Received)



The objectives of this project are to 1) develop a consistent, integrated framework for evaluation of the impacts of hydrogen production within U.S. energy markets using a regionalized version of the MARKAL model; 2) evaluate costs and timeliness of various scenarios of a developing hydrogen supply infrastructure; 3) evaluate the impacts on U.S. energy markets including price and consumption changes for coal, natural gas, renewables and electricity; and 4) identify the most economic routes and financial risks of hydrogen production. The objectives for FY 2007 were to complete regional supply and cost analyses of coal and carbon sequestration, develop regional biomass supply curves, develop fuel and feedstock transportation capacity and cost, perform a study of natural gas infrastructure constraints and costs, and produce and test an initial multi-regional version of MARKAL.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.1** for its relevance to DOE objectives.

- I applaud the efforts of the PI in order to understand the impact not only on resources infrastructure but also on CO_2 sequestration.
- Good alignment with DOE Hydrogen Program.
- It is important to articulate the impact of hydrogen on other alternative fuels as well as to evaluate the impact of other alternative fuels on hydrogen and to compare the impacts of greenhouse gas emissions limits and other "drivers" on all alternative fuels.
- This project is evaluating the effects of the introduction of hydrogen into the energy marketplace on the price and consumption changes for other sources of energy, such as coal, natural gas, renewables and electricity.

Question 2: Approach to performing the research and development

This project was rated **2.8** on its approach.

- The technical approach is based on the well-developed MARKAL model. Extending the model to 10 regions provides the ability to analyze regional differences.
- Important contribution to DOE's overall R&D scope.
- Will be made more powerful by integrating with the Macro System model in the future.
- The approach seems to be very robust and to rely on robust data.
- The approach does not seem to take into account certain very well-known government policies and programs that favor certain fuels, such as tax reductions, tax exemptions for biodiesel or natural gas and such as government subsidies for biomass.
- The approach also needs to take into account that in certain states or regions, there may be localized government policies and programs that favor particular alternative fuels or all alternative fuels. For example, a state may require fleets to participate in the Chicago Climate Exchange or to waive all taxes on alternative fuels.
- The analysis is based on the MARKAL model, actually on a new regionalized version of the model.
- Additional analyses will be based on other databases and models that the PI has.

- There was no explanation of how MARKAL works, so it is difficult to assess what is included and what is not.
- Pipeline delivery from distributed production site may have some advantages and be consider.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.7** based on accomplishments.

- The focus is too much on coal and biomass even though these do not provide major sources of H_2. The presentation did not include details to back up its accomplishments and preliminary findings (e.g., "significant reduction in tax revenue", or "limited impact" on natural gas demand and price).
- Technical accomplishments provide significant progress in addressing an analysis of the coal and biomass markets.
- The PI did not make clear what the technical barriers are that encumber attainment of the objectives of the research.
- The PI did not show how the accomplishments relate to the objectives of the research. For example, having completed the coal resource base, how much more work and what else has to be done to evaluate impacts on U.S. energy markets (objective 3 listed on viewgraph 3)?
- The first set of accomplishments is heavily weighted towards coal.
- The underlying assumption seems to be that bulk of the hydrogen would be produced from biomass gasification and coal, with carbon capture, sequestration, and disposal. Both of these are highly developmental (speculative?) at this stage, so this type of analysis is premature, at least.
- Not clear what is the significance of the "full market penetration" curve on slide 15, and that of the corresponding petroleum products demand in 2050 (slides 16 and 17), since that scenario is totally at odds with the HFCIT and NAS scenarios.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.7** for technology transfer and collaboration.

- This project appears to be working in isolation as compared to DTI, HDSAM and the other systems analysis work presented during this session. It is not clear to me on how this project will interface with other models being developed in other projects in systems analysis.
- Infrastructure design could benefit from consideration of work done by HyDRA and UC Davis and others – appearance is that this is being done in isolation of other potential sources.
- Collaboration with industry is not very evident.
- Good progress has been made in linking the model to sources of data, it isn't clear how the results of this project are linked to other models or making an impact on other related modeling efforts.
- Need to work more with others doing similar work. It seems to me that you are operating in a bit of a vacuum.
- The PI seems to have coordinated the research well with other organizations that are part of DOE or are DOE-funded.
- However, the PI seems to not have collaborated with subject matter experts outside of the DOE community, especially those outside the U.S., such as members of the Intergovernmental Panel on Climate Change or IPHE.
- The project team includes Brookhaven National Laboratory and Power & Energy Analytic Resources (PEAR).
- Not clear what the role of PEAR is in the project.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.9** for proposed future work.

- Next steps are clear and consistent based on the analysis of the preliminary results and project goals.
- It's not clear what is being done to address the barriers listed.
- The plans for future work include examining alternative scenarios and sensitivities without much specificity.
- I don't see any reference to validation or collaborative validation in your future proposed work.
- Plans for future work identified at very high level.

- More details needed on what "finalize data inputs for MARKAL" and "examine integrated scenarios" mean and how these relate to the objectives for the research project.
- The major activities are additional data input and some additional scenario analyses.
- Not clear as to what use would be made of the results.

Strengths and weaknesses

Strengths
- The project is providing useful information on carbon sequestration.
- The project has provided a detailed and carefully thought-out analysis of the issues and impacts regarding carbon capture and sequestration.
- Your incorporation of new technologies for different pathways into MARKAL.
- This project is sorely needed to fill a need.
- Presumably, MARKAL has been used extensively in industry.

Weaknesses
- It was difficult to assess progress due to lack of details. Only general statements were provided. Work seems to have drifted off the objectives.
- Need to work more closely with others to calibrate / validate your model results and assumptions.
- Research project needs to identify areas of high uncertainty and data that have very high uncertainty – such as sequestration. These areas need to be identified upfront and highlighted as visibly as the assumptions in the model.
- Research project needs to include the impact of very highly visible government programs and policies that incentivize certain alternative fuels and their impact on different types of energy consumption, such as tax reductions or tax credits or greenhouse gas emission limits, such as the recent Supreme Court ruling against EPA on interpretation of the Clean Air Act.
- The rationale for the project objectives is not self-evident, neither was it explained in the presentation.
- Used acronyms and abbreviations without explanation (weakness in the presentation, not in the project).
- Methodology was not transparent (at least to this reviewer who did not know anything about MARKAL).
- Model needs to be calibrated.
- Data handling screens appear busy and distracting and should be simplified, similar to Macro-System Model.

Specific recommendations and additions or deletions to the work scope

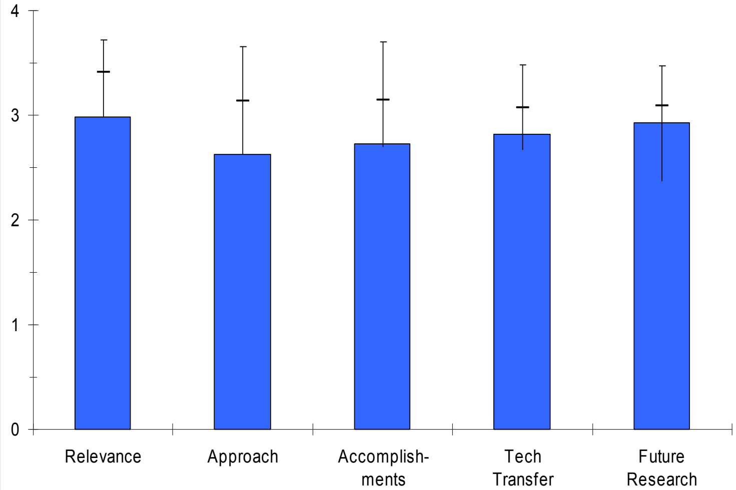
- The project would benefit from more integration with other systems analysis modeling efforts at DOE particularly sharing of inputs and outputs to DTI, HDSAM, etc.
- It appears to me that there appears to be some duplication of the same efforts by other groups within the systems analysis group at DOE, e.g., demand estimates, but I suspect this is not really the case as the estimates are derived from different directions.
- Focus more on the stated purpose of the program and more on typical hydrogen production methods such as SMR rather than CO_2 sequestrations and coal/biomass.
- The weaknesses identified above should be addressed in the future.

Project # AN-03: Analysis of the Hydrogen Production and Delivery Infrastructure as a Complex Adaptive System
George Tolley; RCF, Inc.

Brief Summary of Project

The objectives of this project are to 1) use agent-based modeling to provide insights into likely infrastructure investment patterns; 2) deal with the chicken-or-egg aspect of early transition; and 3) provide an answer to the question, "Will the private sector invest in hydrogen infrastructure?" These objectives will be met by focusing on investments as business decisions, developing a basis for preliminary assessment of profitability, and preparing an agent-based model for detailed simulations.

Overall Project Score: 2.8 (7 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.0** for its relevance to DOE objectives.

- A very interesting approach to transition scenario analysis, i.e., includes behavioral/interaction type analysis between relevant agents and thus may potentially be integrated with the other deterministic economic analysis done by most of the other project teams in systems analysis.
- Better to focus on specific technology, in the short term, that enables the rollout. Expensive program and results will need to be commensurate with cost.
- Complex model, but one that would be a great contribution to DOE's model framework.
- The type of modeling that is the objective of this research is both consumer-oriented and investor-oriented.
- Consumer-oriented modeling is really market research and not a valid, legitimate subject for any government funding.
- Market research is best left to the private sector, which is best suited to do this type of research.
- Investor-oriented research is really financial planning and is not a valid, legitimate subject for any government funding.
- Investor-oriented research is best left to the private sector, which is best suited to do this type of research.
- This project is trying to assess how the private sector might invest in the hydrogen infrastructure as part of the transition to hydrogen as an automotive fuel.
- You are doing a very useful modeling effort that will help vehicle manufacturers, refueling station builders, and users. This type of project benefits many players and it is important that the DOE funds it so that each individual player does not need to build their own models based one more limited data.
- This type of collaboration is an excellent example of a value-added project for multiple participants.

Question 2: Approach to performing the research and development

This project was rated **2.6** on its approach.

- The project would benefit from a better/more complete understanding of the business goals of energy companies such as their risk profiles, attitudes and spending practices rather than assuming certain risk profile/utility curves.
- The project appears to only include capital spending on building fueling stations, i.e., primarily distributed hydrogen generation. A central production with pipeline delivery may alter spending profile of investors. Have the PIs considered this scenario?

- Generally, energy companies spend a very small fraction of the capital budget on station development/construction. Has the PI considered the impact of this on the overall interaction?
- For the task at hand, the approach seems effective.
- Topic is timely, but the model needs to be validated, i.e., get stakeholder buy-in.
- The approach is confusing in that agent is both the consumer and investor.
- The same socioeconomic approach, same investment approach, and same risk approach cannot and should not be taken for both.
- The consumer has totally different motives, values, norms, expectations, and risks from the investor.
- The consumer has a totally different amount of capital to work or play with from the investor.
- The consumer has a totally different capitalization rate from the investor.
- The results of this agent-based modeling would be strongly influenced by the assumptions made about agent behavior and response to various parameters.
- Some of the assumptions about driver agents are not consistent with this reviewer's own (admittedly subjective) feelings.
- Assumptions about the other agents' behavior also do not inspire confidence in the response and the results.
- The model appears to be very subjective. Assumptions are heavy based on the socioeconomic status of people, but weighting is not described or discussed.
- Much of the behavior model is based on perception, education, communications and patterning. As such, the model is lacking factors such as the education and training of the population, and safety, utilizing current local infrastructure. (Integration with Hydra would help).
- Model needs to list all input factors and prioritize or weight them in some fashion. More thought needs to go into input parameters.
- This is not least cost optimization but modeling behavior of agents – agent-based modeling; takes each individual agent and models his behavior.
- This modeling approach takes into account feedback from customers and response by suppliers, incrementally over time. This approach is extremely useful for modeling incremental fueling station adoption.
- Please show the different in revenue streams (or profits) to vehicle sellers with slow versus fast learning.
- Please show the difference with an initial government fleet adoption into an area (LA county police gets H_2 cars).

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.7** based on accomplishments.

- It is personally difficult for me to assess overall value while only considering distributed infrastructure in this model. Also the investor risk profile of auto OEMs has not yet been incorporated in this model.
- The focus of the presentation concentrated more on consumer purchase of vehicle as opposed to decision by an infrastructure provider.
- Very tough topic to tackle. I commend you on your work, but need to stress again that validation is key to making this a useful model.
- Effect of consumer learning was quantified.
- However, it is *not* clear what consumer learning is required. What is so different about driving a conventional car from driving a fuel-cell car that a driver must learn?
- Second, economics is a much greater driving force or factor than consumer learning. Nowhere does the research seem to take into account the base price of a fuel-cell vehicle in market penetration or market share.
- The significance of the results of sensitivity to parameters is not well explained. For example, it is not clear what is meant by "Consumer Learning Behavior." In any case, for a 50% hydrogen vehicle sales share, there is a difference of only 8 years between the extreme cases considered.
- No vehicle production constraints appear to have been considered.
- The investor risk aversion cases examined show only a 2-year difference for 50% of vehicle sales share.
- Other results presented are strongly influenced by the assumptions, some of which were not transparent.
- New project understand results preliminary.

- You stated that you are assuming a risk return rate borrowing rate of 12% which is constant over time. My impression is that this rate of return is too low for the level of risk being taken on by investors and consumers. It should probably start out high and then decline over time as people's perceived risk changes.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.8** for technology transfer and collaboration.

- I see a good list of project partners/advisors but I am concerned over value of their contribution since some assertions don’t seem to be valid, e.g., investment levels by major energy companies.
- The presentation did not elaborate on interaction with the private companies listed and it's not clear if their input is included. This is important since they are the ones being evaluated on whether they will invest. Need input from them on what risk they might accept.
- Could also interface with other Analysis projects evaluating infrastructure rollout options to minimize risk.
- Would recommend that you work closely with OEM's to validate your model against either Diesel breakthrough in Europe over the past 30 years and or hybrid breakthrough here in the US over the past 5 years.
- The research focuses on the chicken-egg problem nature between hydrogen fuel infrastructure and hydrogen vehicle market share.
- The research project fails to coordinate with, collaborate with, or take advantage of other research done on the chicken-egg problem solving done by Argonne National Laboratory, namely in project ANP-3, "System Dynamics: HyDIVE — Hydrogen Dynamic Infrastructure and Vehicle Evolution Model."
- The project team includes companies, universities, and research laboratories.
- It is not clear how involved the other partners are in the actual research being conducted.
- This project could use a team of collaborators to vet the input parameters. Team should include modelers, oil companies, auto companies, behavioral psychologist.
- The project is working with Ford Motor company closely and Argonne National Labs and companies (BP, Air Products) and University of Michigan.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.9** for proposed future work.

- Next steps are clear and aligned with project goals.
- However, it is not clear to me from the presentation whether the interaction of auto OEM will be captured in future work?
- There was no clear approach to how to overcome the barriers listed, such as lack of good data.
- Future plans are discussed at a fairly high level with very little detail.
- The model fails to make important distinctions in the types of agents and their values, norms, expectations, risks, and the amount/type of capital. Unless the model is revised in the future to take those distinctions into account, it is of little value.
- Future work will further expand the model to include additional production and delivery options, additional agent behavior patterns, and market structures and incentives.
- Please take the time to collaborate with integrating your model into the Macro-Systems Model.
- Please expand the model to answer some of the additional questions mentioned here.
- Please meticulously document all assumptions and data sources in the model so that others can use it correctly and integrate it consistently with other models.

Strengths and weaknesses

Strengths
- Extremely interesting; and uncertainty and consumer learning parameters are very well captured.
- Interesting data on factors to speed adoption.
- If properly validated, to the point where stakeholders accept the results, this would be a great tool to investigate different roll out scenarios and may even be a learning tool for policymakers.

- Research project considers effect of government incentives.
- With proper input parameters considered and prioritized, this could be a very good predictive model on how people will respond to new or disruptive technologies.
- They got more funding this year, which enabled them to expand the model.

Weaknesses

- It is not very clear as to how this project integrates with other systems analysis project (such as HDSAM, DTI, etc.).
- No discussion on liability affecting private sector investment, or how to get over initial low return of capital and how rollout of different technologies can impact investment decisions. Relative impact of fuel price on adoption (compared to the factors shown) would be helpful.
- No validation.
- More collaboration with OEMs and energy companies to understand the tradeoffs between fuel station availability and vehicle cost.
- Research project fails to distinguish the major differences between the two types of agents: consumer and investor.
- Research fails to take into account the base price of a fuel-cell vehicle and realize that this is much more important than the learning behavior of the consumer.
- This agent-based modeling is very sensitive to the assumed agent behavior.
- The set of assumptions used appears to be incomplete, at the very least.
- Not enough background information was provided to explain or justify agent behavior and response.
- No discussion of how the model results can be used, and by whom.
- Model as it stands is too subjective. It appears to heavily weighted to bandwagon affects and does not take into account economic inputs such as changes in the price of commodities, an expanding or contracting economy, local hydrogen infrastructure influence on build-out, state and local government incentives, training programs. Model needs to be calibrated against some new technology penetrating the market.
- Please document all assumptions in the model meticulously with extensive documentation.

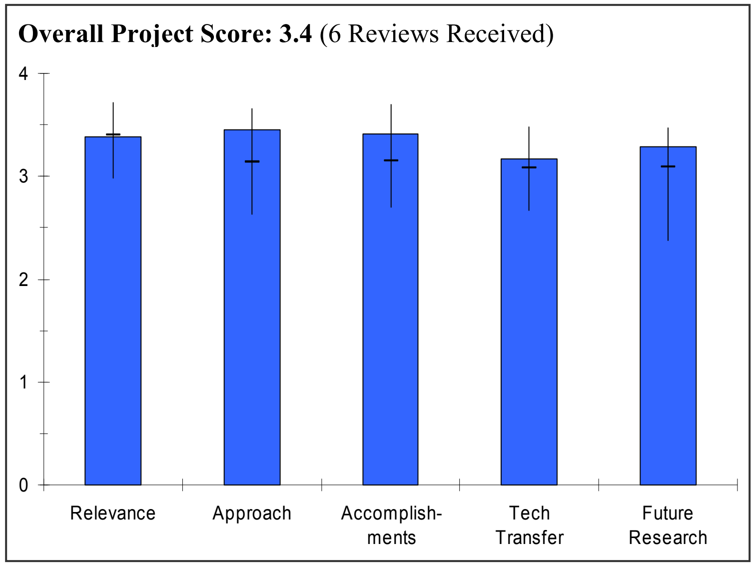
Specific recommendations and additions or deletions to the work scope

- Develop a clear and explicit interaction with other systems analysis teams – DTI, HDSAM, Macro System Model, etc.
- Develop recommendations that can speed private investment in hydrogen infrastructure since that is shown by the results to be important to consumer acceptance. Could the ABM be validated by comparison to the existing gasoline infrastructure?
- I would *not* recommend continuing to work on this model or any model that is consumer-oriented or investor-oriented or any model that examines consumer-investor interaction.
- Profit maximization for a company is a common, useful assumption. Business school literature hypothesizes that companies do not always act to maximize profits but rather employees who work at companies try to maximize their own gains. A simple example is frequent flyer miles – an employee may choose the flight that does not maximize profits for his company but rather gets him the most miles. Have you considered modeling this personal-profit maximization within companies involved with hydrogen which could increase or decrease adoption rates? Is there a frequent flyer equivalent with hydrogen that could increase adoption rates? Expand the model to answer these questions.

Project # AN-04: HyDRA – Resource Analysis
Johanna Levene; NREL

Brief Summary of Project

HyDRA is a web-based geographic information system (GIS) tool to allow analysts, decision makers, and general users to view, download, and analyze hydrogen demand, resource, and infrastructure data spatially and dynamically. Functions of the tool include the following: generate generic viewing maps, resource maps, infrastructure maps, and demand maps; layer control; change underlying assumptions; build hydrogen system; buffer layers; security; import data; export data; select data; and print map. Emissions maps, temporal functionality, and interaction with other applications are also planned.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.4** for its relevance to DOE objectives.

- Project aligns with the need to understand the potential for H_2 production from renewable resources.
- Interesting model, but it's not clear how much use it would be to actual rollout of infrastructure. There are other un-quantifiable considerations that are likely to take precedence.
- Project is aligned with the Hydrogen vision and when validated will serve as an excellent tool and guide for federal managers.
- Companies and investors may use their own models to make decisions, but it is very likely that they will turn to a model such as this to check/verify their decisions.
- Will be an excellent planning tool for federal managers and decision makers.
- This research project seems to make sense even if the DOE RD&D objectives did not exist.
- The project makes sense because it matches resources (renewable) with hydrogen production and the places of demand.
- This project will make hydrogen demand, resource, and infrastructure data available to users.

Question 2: Approach to performing the research and development

This project was rated **3.5** on its approach.

- Approach benefits from previous software development and GIS experience at NREL.
- It seems more like data presentation than a model, but that data is useful to document in one location.
- Utilizing the ongoing NREL models and providing the link to bring them together for H_2 evaluation is an effective use of resources.
- Effectively looking at the competition for resources, at least on a spatial basis.
- Project makes use of available resource databases – wind, solar, biomass – and geospatial locations of these resources.
- Project results in a tool that will be publicly accessible on the World Wide Web.
- Use existing data resources to perform analyses, subject to multiple constraints and drivers.
- The presentation provided a comprehensive overview of the model's capabilities.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.4** based on accomplishments.

- Project has developed an interesting tool in just one year's effort.
- Progress seems on track to meet objectives.
- One of the better presentations and programs with regard to showing actual work and progress.
- Most functional requirements have been met.
- Case study demonstrates good functionality of the model.
- PI did not identify technical barriers.
- The reviewer does not think there are any major technical barriers to overcome for this project to progress to completion.
- It is primarily a model development activity so far.
- Allows simultaneous view of several parameters.
- The case study example showed how the Minneapolis area satisfies the input parameters.
- It is not clear how well hydrogen-fueled vehicles can be related to the parameters in the model.
- Great progress has been made with this new project.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.2** for technology transfer and collaboration.

- Transfer of this model is obvious, because web-based.
- It seems like a tool that will have use beyond this web application. As the MSM is developed, this tool should be useful.
- Several references were made to interactions with other studies.
- Could benefit from input from industry to evaluate its use.
- Technology transfer considerations are excellent when considering that the model will be a web-based system and will be available to (essentially) everyone.
- Collaborations could be strengthened by pulling in business/industry/investment community and determine what they require.
- The reviewer is of the opinion that no additional coordination or collaboration beyond what has been done is necessary.
- However, the project could benefit from seeking users, such as state hydrogen program managers or fleet managers, to evaluate the application.
- At this early stage of the project, there is little technology transfer or collaboration.
- The PI is seeking beta testers to help improve the model and its user interface.
- Would be useful to work with others in GIS area to expand out capabilities and verify model, troubleshoot.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.3** for proposed future work.

- Future research is just finishing the release and incorporating experience from beta users in the rest of this FY.
- Temporal functionality is questionable, given that this should be incorporated into the MSM, which will provide the temporal integration and variations.
- Good details presented on next steps.
- Looking for H_2-knowledgeable people to do the beta testing and this will provide excellent feedback for improvements to the model.
- Another audience to target for beta testing is the intended user of the model, such as the decision makers. It is recognized that many of their comments may not be easily incorporated in the remaining performance period, but might provide good insight for follow-on activity.
- Future plans discussed in sufficient detail.

- PI identified weaknesses in that NREL does not have a good handle on data concerning non-renewable resources and will seek out sources of such data.
- The proposed future activity is primarily model development.
- It would be helpful to show examples of the effective use of the model, such as for helping to guide related research.

Strengths and weaknesses

Strengths
- Project was a good idea as formulated from existing NREL tools and software experience.
- Inexpensive and short term…to-the-point. Good return for cost.
- Fast paced and seeking real feedback.
- Actual work is being shown and demonstrated.
- If underlying assumptions can be validated, it may be an excellent tool for Federal Managers to use.
- Matching of resources and demand.
- Publicly accessible on World Wide Web.
- Flexible model with an easy-to-use graphical interface.
- GIS mapping of resources and population is a strong planning tool.

Weaknesses
- Data will need to be updated for long-term effectiveness.
- Need better plan for validation of model, actively seek industry input.
- To be of most benefit to federal decision makers, this model must closely match the results of similar private sector models. A validation activity should include a determination of how well it does match business/investor decision models.
- PI needs to be more aggressive in soliciting users to test and evaluate the application.
- Need to show how the results can be used effectively.
- Comment (not weakness): the presentation was very fast, rushed, almost breathless.
- None. Understood it is new project.

Specific recommendations and additions or deletions to the work scope

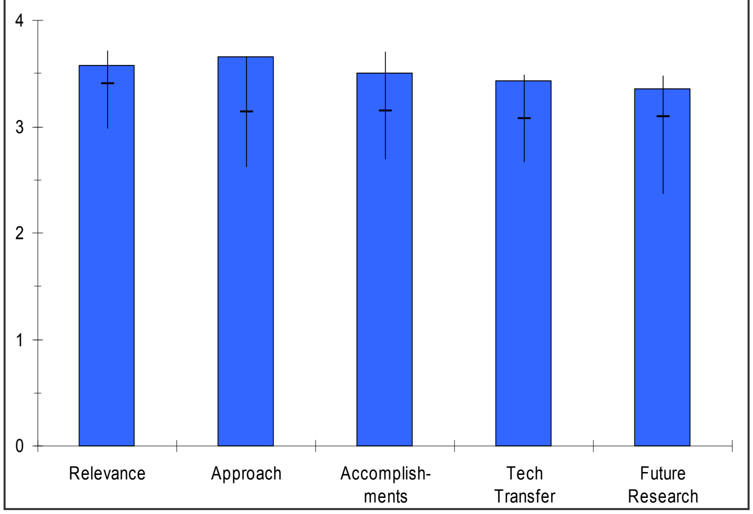
- PI mentioned plan for incorporation of this tool into the MSM; this should be the highest priority.
- Bring in business/industrial decision makers and determine their requirements.
- Not within the scope of this activity, but a potential follow-on activity would be the validation of this model.
- Beta test will very likely bring out priority issues that should be addressed within and beyond the scope of this project.
- Reviewer would like to see the inclusion of EPA map of Clean Air Act National Ambient Air Quality Standards non-attainment areas on the demand layer side of the application and FHWA map of corridors of freight movement congestion (these are major generators of diesel particulate and NO_x, and even if the commercial vehicles are not moving, these are major generators of diesel particulate and NO_x during idling) on the demand layer side of the application. The FHWA map does not necessarily duplicate the EPA map but takes into account sensitivity of town and communities to mobile (commercial vehicle) sources of pollution that could be replaced to a certain extent by non-polluting hydrogen energy.
- Consider adding sites for potential geologic storage of Hydrogen as well as hydrogen pipelines.
- Would be useful to add tool to integrate future weather scenarios and their impact on natural resource development.

Project # AN-05: Macro-System Model
Mark Ruth; NREL

Brief Summary of Project

The overall objective of this project is to develop a macro-system model (MSM) aimed at performing rapid cross-cutting analysis within the Hydrogen Program. It uses high-level architecture to link models being developed or used by the Program. The MSM supports decisions regarding programmatic investments and focus of future funding through analyses and sensitivity runs. It also supports estimates of program outputs and outcomes. Currently, the H2A, HDSAM, and GREET models have been linked within the MSM framework.

Overall Project Score: 3.5 (6 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

- The purpose and relevance are clear – there is obviously a need to integrate several "disconnected" models into a combined value chain approach.
- If these models are being developed, it makes sense to make sure they are consistent and can be used together.
- Clearly there is a very serious need to link models together to get a more uniform and consistent output, this model will do that.
- The macro system model (MSM) is a "master" program that can call up and use a library of existing models developed at NREL and elsewhere.
- If successful, this project will be an important tool for System Analysis and the overall program to assess the benefits and costs of a future hydrogen economy.

Question 2: Approach to performing the research and development

This project was rated **3.7** on its approach.

- While the approach towards integration appears strong, MSM heavily relies on H2A, HDSAM and GREET. Perhaps including a feedback loop from MSM to validate/challenge the other models' assumptions and results may also be a beneficial approach as part of the future work.
- The current version of the model is deterministic, which is okay to start with. However, for an emerging technology such as hydrogen, a stochastic approach needs to be taken and I hope MSM considers adopting this approach soon.
- Well laid-out plan.
- Model has a good, simple layout for a complex subject.
- Excellent approach to linking existing models via currently selected simplified architecture.
- Linking existing models via an overarching Federated Object Model, so that the user does not have to call up individual models.
- I would have liked to have seen more presented on the approach in the oral presentation, but the PI covered some of the details during the demo session.
- The current linking approach appears to be suboptimal, but the team is appropriately trying out an alternative solution.
- The team is taking the right approach by starting small and building over time.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.5** based on accomplishments.

- PI demonstrated clear progress and accomplishments in capturing the types and category of information needed. I do see clear value in the model integration efforts of MSM. However, the overarching goal for the systems analysis teams of DOE interfacing with MSM is not completely clear to me because this presentation (and previous presentations in the session) did not clearly outline what the main objective of the systems analysis teams models, i.e., what are we trying to achieve via integration – is it policy planning, is it investor analysis, etc?
- Preliminary sensitivity analysis and tornado charts are good indicators of integration of several models.
- Presentation offered actual results, showing the model is at least functional, if not yet validated.
- Excellent progress from last year.
- Developed and validated interfaces with many separate models.
- Added several more pathways this year.
- Valuable side-effect of the project is vetting current models.
- An important challenge will be de-bugging since it involves data transfer between various models.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.3** for technology transfer and collaboration.

- While collaboration of MSM with H2A, HDSAM and GREET have been well recognized, I encourage the PI to interface more with DTI and RCF in order to include scenario analysis.
- Good input from other labs, but need more input from hydrogen producers/users.
- The collaborations are mostly with the developers of the other models that are being interfaced with the MSM.
- There appears to be sufficient collaboration so far with the necessary model developers.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.3** for proposed future work.

- Next steps are clear and concise.
- Well laid-out future steps and plan in presentation.
- Good plan forward, validation is key as is providing a more user friendly GUI.
- Future work is primarily an extension of the model.
- Ambitious, but reasonable plan for future work.

Strengths and weaknesses

Strengths
- Integration of several models in a single location – production, delivery, emissions.
- Well organized, good plan, and good progress.
- Allowing for one top-level layer to interface with other models to provide consistent assumptions to be used throughout will help to compare model results more easily.
- Makes several different models available simultaneously in a "one stop shop".
- If successful, this project will be an important tool for DOE to make the right R&D and planning decisions. However, the project will only be as good as the models it interfaces with.
- Broad-based modeling linking emissions to production and delivery scenarios.

Weaknesses
- No major weakness as such; however, the project is heavily reliant on the accuracy of the other models. Therefore, I am concerned with the error propagation from the other models. Does MSM test or challenge the assumptions of other models?

- This project has similar issues as other models in how to account for intangibles and unquantifiables.
- User interface at this point is not so great.
- Would have been helpful if the different models used in the case studies were listed.
- Did not explain what we were looking at in slides 13-17, each of which had the same title.
- How do we use this information?
- It was not clear how this is an advance over using GREET or H2A, for example, by themselves.
- Is MSM interfaced with H2A?
- It isn't clear yet how the analysis community will be able to utilize the model to answer questions, but I assume this will worked out in the future work (i.e., beta testing).
- Very ambitious, perhaps too ambitious, end goals (i.e., individual models still need to be developed and utilized).
- Model needs some control to be calibrated to determine degree of error in calculation. Can this be applied to actual plant operation to determine accuracy?

Specific recommendations and additions or deletions to the work scope

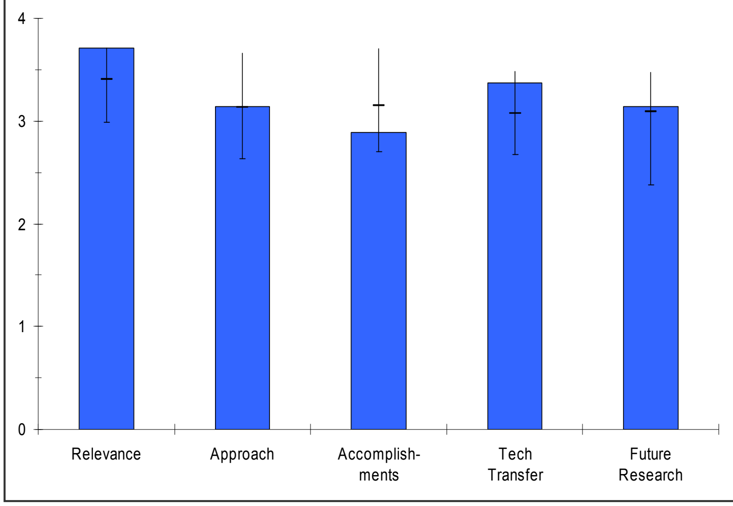
- Develop a clear and concise plan to handle various revisions of H2A, HDSAM, GREET, etc. into MSM.
- Include a methodology to challenge/validate assumptions and results from the above models (which are inputs to MSM).
- Add H_2 quality/cost tradeoffs into MSM.
- Add stochastic modeling capability to capture uncertainties.
- Need to make assumptions clear and adjustable to user.
- Transition scenarios (in future work) should be thoroughly vetted by industry (e.g., auto OEMs and energy companies).

Project # AN-06: Hydrogen Quality Analysis: Production to Fuel Cell
Romesh Kumar; ANL

Brief Summary of Project

The DOE Hydrogen Quality Working Group (HQWG) is tasked with developing a process to determine hydrogen quality requirements for fuel cell vehicles, based on life-cycle costs. This project will identify how fuel quality influences the life-cycle costs of the various components of the overall "hydrogen system" and will develop models to evaluate the effects of fuel quality on the costs of the hydrogen system components. The HQWG will also identify information gaps and the research and development (R&D) needed to fill those gaps.

Overall Project Score: 3.2 (7 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.7** for its relevance to DOE objectives.

- Understanding cost effect of impurities on FC vehicles is relevant.
- Hydrogen purity is a very important parameter to rolling out hydrogen as a fuel. It is currently a very controversial topic that needs to be resolved and is potentially a roadblock unless resolved.
- Very, very important topic!
- Very high relevance.
- The project complements other efforts in fuel quality, determining the consequences (mostly monetary) of impurity tolerance specifications.
- Tighter tolerances add to the cost of fuel, and analysis is necessary in order to prevent these added costs from exceeding the costs of damage that the impurities might cause, or the costs of remediation methods that might make the system tolerant of such impurities.
- The project is necessary to bring together the future hydrogen producers (e.g. energy companies), developers (e.g. fuel cell and hydrogen systems) and end users (e.g. auto OEMs) to help establish the least-cost approach to hydrogen quality.

Question 2: Approach to performing the research and development

This project was rated **3.1** on its approach.

- Approach includes a physical model of PSA systems to understand cost of impurity concentration.
- The approach of using the lowest $/mile is a good one, but the focus of the presentation (and work performed to date?) seems to focus on hydrogen cost rather than fuel cell life.
- We have two very competent and experienced PI here, why are there no experiments to validate some of these numbers presented in the findings.
- Integrated approach is very good.
- Gap identification for resource allocation is a key element.
- The project utilizes a team approach to gather, critically assess, and integrate relevant data.
- The approach includes data gathering, model development, a good degree of communication among team members, and ultimately development of a roadmap to steer the community towards the least-cost architecture for dealing with fuel impurities.

- Important outcomes of this work are the identification of (1) information gaps as to the actual costs caused by fuel impurities or measures taken to remove them, and (2) areas of useful R&D that could lead to reduced system costs.
- Balancing cost of FCV and H_2 is a great idea, one that has not yet been fully studied.
- It is not clear how this project is coordinating with industry representatives outside of the FreedomCAR Tech Teams.
- Why consider an ATR for natural gas reforming? Are any developers still considering ATR over SR?
- Modeling PSA may be a waste of time as the industry should already understand the performance trade-offs.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.9** based on accomplishments.

- A model is started, but initial results look simplistic.
- There was little or no data presented that discussed the impact of purity on fuel cell as opposed to cost of hydrogen. It was mentioned, but could be discussed further.
- Summary items match well with reality, which is a good sign.
- The level of confidence in the data is not presented. Too bad there are no field work or lab experiments to support the information presented. It would be great if the PI can conduct some sort of sanity check on the information gathered.
- The project is beginning to bear fruit in such areas as analysis of the costs and effectiveness of steam methane reforming (SMR) and pressure swing adsorption (PSA).
- The PI reports that a "comprehensive draft Roadmap" is out for comment.
- The PI did not make clear whether or not they consider the data gathering phase of the project substantially done, that is, whether all the data (or sufficient data) actually exists within the project in order to make the draft Roadmap truly "comprehensive."
- The project seems to have spent a lot of money with no real results to date.
- It is not clear what has actually been accomplished besides a literature review and getting up to speed on H2A.
- Cost curves presented appear to be based on previous work (i.e. lit review).

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.4** for technology transfer and collaboration.

- Excellent collaborations with industry partners on supply and vehicle sides.
- Good number of partners in oil and automotive industries. The group could use representatives from hydrogen and analytical industries as actual participants.
- Keep up the good work.
- Accessible library database of focused content will be important in focusing needed research.
- Very good cross-functional collaboration.
- Performance degradation models will be helpful in the development of a hydrogen quality standard.
- The presentation indicated many proactive efforts to gather detailed data from various sectors and to report findings in a timely manner.
- The questions at the end of the talk indicated a high level of interest in the community on this activity.
- The consensus standards bodies currently working on fuel-quality standards (principally SAE, ASTM, and ISO TC 197) are "open" – meaning that all interested and affected parties may participate. While the H2QWG seeks participation from all sectors, it should be more "open" in the same sense – allowing, soliciting, and welcoming participation by any and all interested and affected parties.
- Not enough fuel cell and hydrogen component developers have been engaged (e.g. on the fuel cell side, only UTC and Ford to date – Ballard has provided some info).
- Need more review and input from industry outside of the Tech Teams.
- There has been no information shared with the public on this project until this Merit Review.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.1** for proposed future work.

- Plans to update model with data.
- Good list of future action items.
- Access to good data on fuel cell performance was not listed as a barrier. If available, this data could be included as well.
- PI needs to propose some sort of field or experimentation to check on the information. The information gathered so far does not have a high level of confidence or buy in from all industry members. How do you plan to validate the model?
- Future research and model development should be more closely focused on DOE goals for catalyst loadings
- The PIs propose to further polish their model (build and validate), publish an initial roadmap, publish a roadmap, and otherwise continue with their well-laid plans.
- It would be good to not rely entirely on model results, but rather have a healthy combination of model results and OEM validation.
- There is no end date for this project?
- It is not clear what final outcome is desired/expected.

Strengths and weaknesses

Strengths
- Collaborations in the working group should provide insight into the question of what H_2 quality is necessary and cost-effective.
- This project is addressing a critical issue and has a reasonable approach.
- Very good PI focused on a major issue at hand.
- Project Strength lies in its cross-functional depth.
- The project complements other efforts to determine the effects of fuel contaminants on fuel cell components, and to set standards for fuel purity.
- In the presentation, the PI well articulated a sensible scope and course of action for this activity, providing value without overreaching into areas already covered by others.
- This project seems well coordinated with other efforts concerning fuel quality.

Weaknesses
- I'm not sure how this project fits in with the other analysis projects. Unless the PSA model will have utility elsewhere, it appears that this project might fit better in the FC program.
- It will be difficult to drive to a consensus.
- It's not clear why the focus is on production (in short term to 2015) when delivery of liquid/gas is likely to be the biggest supply mode in this short term.
- Validation of models will be critical.
- The working groups should be open to all interested and affected members of the community.
- Additional clarity should be given on the extent to which the first roadmap will be "comprehensive," or to the extent that subsequent roadmaps will build on data not yet in hand.
- This is the first time the public has seen anything from this project, and even now, there are no substantial results to speak of.
- Not much progress given the level of funding.

Specific recommendations and additions or deletions to the work scope

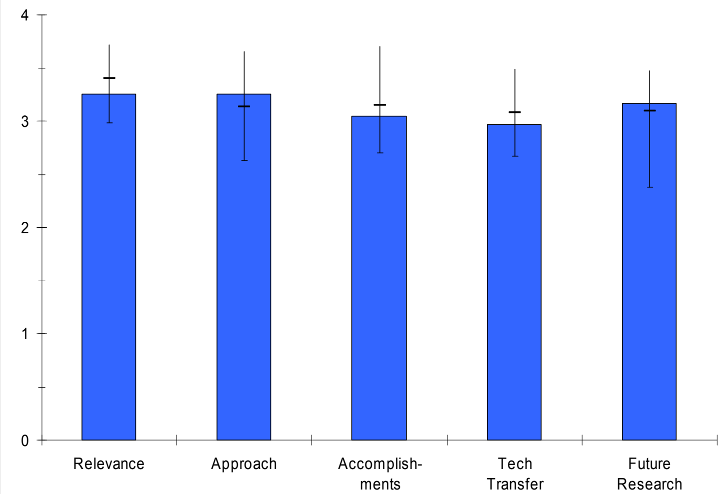
- Consider cost of cleanup on vehicle vs. at a station or at production.
- Include particulates as a contaminant for discussion.
- Should consider conducting some sort of field work or lab experiments to support findings.
- Direct future work to verify current models with DOE targets.

- ANL should focus on the fuel cell performance modeling and work with fuel cell cost analysis teams and hydrogen production and delivery teams for the cost trade-off assessment.
- Need more collaboration/coordination with industry outside of Tech Teams (e.g., fuel cell and hydrogen system developers as well as other analysis teams).
- Need to get more results soon and have an end date.

Project # AN-07: Well-to-Wheel Analysis of Hydrogen Pathways with GREET Model
Michael Wang; ANL

Brief Summary of Project

Overall Project Score: 3.1 (6 Reviews Received)



The objectives of this project are to 1) expand and update the GREET model for hydrogen production pathways and for fuel cell vehicle improvements; 2) conduct well-to-wheels analysis of hydrogen fuel cell vehicles with various hydrogen production pathways; 3) provide well-to-wheels results to assist in DOE planning and evaluation activities; and 4) engage in discussions and dissimilation of energy and environmental benefits of hydrogen fuel cell vehicles. Major efforts in the last year included well-to-wheels analysis of energy use and greenhouse emissions for selected hydrogen production pathways (distributed production from natural gas via steam methane reforming, central production from cellulosic biomass via gasification, central production from coal via gasification with CO2 sequestration, distributed and central production from wind/grid electricity via electrolysis, and central production from nuclear via thermo-chemical water cracking), and analysis of potential energy and greenhouse gas emissions effects of hydrogen production from coke oven gas in U.S. steel mills.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

- Well-to-wheel analysis is important to understanding emissions and benefits of H_2.
- The analysis is helpful to compare different roll-out strategies for the hydrogen economy.
- It is absolutely essential that this (and other) activity maintain awareness of greenhouse gas and emissions impacts that are likely to result from the future deployed technologies.
- It is not clear why this project is focused on hydrogen end-use as fuel cell vehicles.
- It is not clear what the practical application of the results of this research project are when the choices for hydrogen production methods may be constrained, such as by geographic proximity to renewable resources.

Question 2: Approach to performing the research and development

This project was rated **3.3** on its approach.

- GREET is a well documented tool in W-T-W analysis; it makes sense to adopt H_2 pathways for comparison with other alternative fuel options.
- The original choice of a spreadsheet as the choice of platform limits the potential future uses somewhat.
- The project is continuing to refine an existing model.
- Expanding credible model. This approach is outstanding and takes full advantage of more than a decade of prior research and model development.
- Looking at all of the right sources for data. The data sources being used are all of the reasonable sources that could be suggested. The fact that they are getting anything from industry is commendable.
- The PI needs to interface with energy providers too; they deal with quite a bit of hydrogen daily. What about obtaining the data on the FCVs from the Technology Validation Program?
- Project makes use of available resource data bases.
- Project results in a tool that will be released to users.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- The results presented here are skewed by the overly optimistic assumptions regarding FC vehicle mileage, in comparison to the overly pessimistic assumptions for the mileage of a hybrid gasoline vehicle. The authors chose a range of 35-39 mpg for a gasoline hybrid, when the Prius is EPA rated at 55 mpg (composite mileage) and on-road is about 45 mpg; the authors adjusted down from a Prius for vehicle size. In contrast however, the FC vehicle is assumed to get 55 to 65 mpg, which is extremely optimistic compared to the values measured as part of the Technology Validation vehicle learning program (see Wipke, TV5). The author mentioned Honda FCX, which has EPA rating similar to Prius (within 1 mpg), yet somehow the FC vehicle's mileage is adjusted upwards under the argument that these prototype vehicles are not representative. These optimistic assumptions dominate the comparisons to follow.
- Another example of overly optimistic input assumption is the >80% efficiency in NG reforming assumed for 2015; this maybe related to a DOE target, or come from assumptions built into H2A, but there is no evidence that the technology will get there.
- The authors do not consider sensitivity studies on any of these parameters to evaluate how critical the assumed values are to the outcome and conclusions.
- The GREET project continues to be a common platform used extensively for analysis.
- Fabulous list of H2 production pathways already included in the model. This could not have been accomplished without the prior research that had gone into GREET.
- PI needs to show levels of uncertainty in the numbers presented so it will be easy to understand the levels of accuracy. These numbers cannot be absolute.
- PI identified technical barriers as inconsistent data, assumptions, and guidelines. However, PI did not explain the details of these inconsistencies.
- PI should show the variation (upper bound and lower bound) or uncertainty in outcome(s) of the GREET model as a result of these inconsistencies.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- Author makes GREET tool available.
- The GREET project has gotten input from various sources, but it has not been discussed how consensus is reached on the assumptions.
- This is the right team for development of this model.
- Inputs are being collected from the right organizations and sources.
- GREET's credibility has lead to a user list that total 3500. As the H_2 pathways are added, they are available to these and additional users.
- PI needs to interface with the Fuel Cell Tech Team, Hydrogen Production and Delivery Tech Team, along with energy providers.
- Though your current partners are full partners and apparently are full participants, it would be useful for the future development of the model to work with industry to get real validation/comment on your model results.
- The reviewer is of the opinion that no additional coordination or collaboration beyond what has been done is necessary.
- However, the project could benefit from seeking feedback from users,

Question 5: Approach to and relevance of proposed future research

This project was rated **3.2** for proposed future work.

- Several next steps are laid out.
- Agree with current plans for expansion of the model. Would recommend that plug-in hybrid fuel cell vehicle be added to the mix.

- PI needs to collaborate with companies like Air Gas to get decent numbers on trucking of hydrogen costs and other tech team to get accepted numbers in his proposal.
- The implementation of a full lifecycle analysis would be very useful to help understand the GHG emission for different scenarios.
- Future plans discussed in sufficient detail.

Strengths and weaknesses

Strengths
- The GREET tool is a useful contribution to the analysis community.
- GREET is a large multi-faceted model that is developing consistency for this type of analysis.
- Building on one of the most credible and used models in the DOE system.
- Good overview of simulation.
- Excellent program – really helps me understand well to wheels and well to pump results.
- GREET model has become a standard Wells-to-Wheels analysis tool.
- GREET model used for DOE Hydrogen Posture Plan.

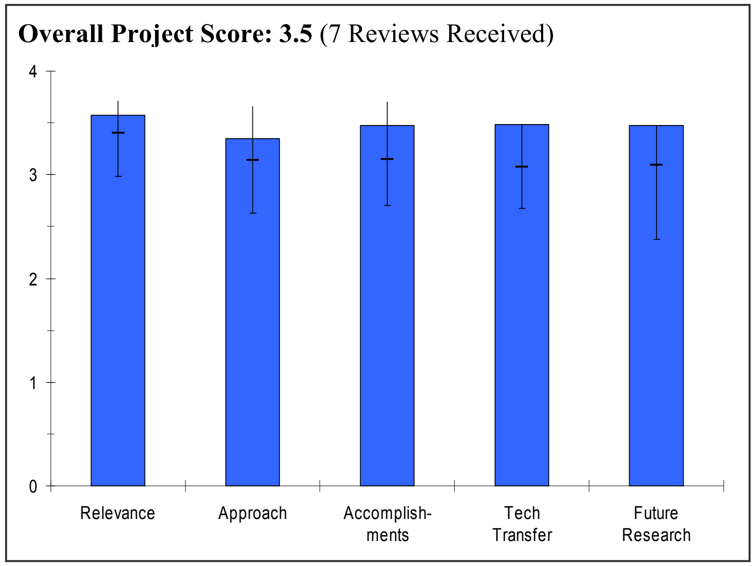
Weaknesses
- The model is only as good as its assumptions. It's important to continually update those assumptions and provide visibility on the process of how they are determined.
- Need to consider current consumption of the hydrogen and how will the increase in demand affect the overall cost of hydrogen. PI needs to show standard deviation to show accuracy of numbers.
- In future it would be great to have more of a life cycle analysis incorporated into the model, to allow for GHG analysis.
- PI needs to solicit feedback from users on improvement and enhancements.

Specific recommendations and additions or deletions to the work scope

- The author needs to provide a parameter study using the critical assumptions.
- Provide more detailed objectives each FY as model is continuously refined and improved.
- Add the plug-in hybrid fuel cell vehicle to the technology options that are modeled.
- PI needs to interface with all the stake holders of this simulation work (FCTT, H_2 Production and Delivery, Energy Providers, etc).
- Implement a means for soliciting feedback from users.
- Take into account (in terms of impact on hydrogen production efficiency, energy use, greenhouse gas emissions, etc.) the estimated energy needed to sequester carbon that may result from hydrogen production methods that rely on fossil fuels, such as hydrogen from coke-oven gas.

Project # AN-08: HyTrans Model
David Greene; ORNL

Brief Summary of Project



Oak Ridge National Laboratory has created a working version of an integrated model of the market's transition to hydrogen as a transportation fuel using non-linear optimization methods. The model includes representation of 1) hydrogen production and delivery; 2) vehicle production, including technological progress, scale economies and learning-by-doing; and 3) demand for vehicles and fuels, including the effects of fuel availability and diversity of vehicle choice. The objectives of this project in FY 2007 were to complete development of an integrated market model of the hydrogen transition (incorporate reduced form representations of the H2A production and delivery models, develop new fuel cell vehicle cost model, add regional detail) and to use the HyTrans model to describe and analyze DOE's early transition scenarios (2012 to 2025) and publish a report on their costs, benefits in greenhouse gas (GHG) and oil reduction, and sustainability beyond 2025.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.6** for its relevance to DOE objectives.

- The analysis uses program targets and evaluates the proposed FCV sales scenarios using a model of market effects on driver choice and H_2 supply.
- Successful transition and evaluation of how to get there is important to understand if a hydrogen economy is possible.
- This project is highly relevant and focused on the overall DOE objectives. It is less about creating a model, and more about actually using the model to address the key questions and key sensitivities.
- This is one of several models that are addressing the issue of transition to a hydrogen transportation system and infrastructure.
- This is a relevant issue but virtually impossible to execute in a meaningful (relevant) manner.
- It isn't clear that the results of this study, as conducted, will have any effect on the program regardless of the results.
- This type of model is important for developing well-to-wheel estimates of energy and emissions.
- The future of this model should be enabling users to have more control over input parameters (such as efficiencies, emission factors, etc).

Question 2: Approach to performing the research and development

This project was rated **3.3** on its approach.

- The approach of using market, even with the efficient market assumption, is valuable to understand how the transition to hydrogen might occur.
- The fact that the "no scenario" run of the model predicts no market for FCV is reassuring, in that it reflects the realistic fact that there is a hurdle to public purchase of these vehicles.
- One of the barriers has to be the quality of the cost data, but this was not addressed specifically.

- The model is well-designed and adaptable to DOE program needs. It draws information from a wide variety of sources, and doesn't try to duplicate existing models.
- Excellent approach.
- Uses/incorporates various existing models.
- Incorporates new vehicle cost data from OEMs.
- The approach is generally good given the real limitations on such broad modeling. But, the approach is generally assumption driven (as it must be) but too many of the assumptions are unrealistic. A better approach would probably be one emphasizing a sensitivity analysis for the more critical (and questionable) assumptions.
- Too many of the important components of the models used in the approach were either glossed over or neglected completely, thus making an assessment very difficult. It is recognized that there are time limitations, but additional information could have been included in the slides even if there was not time to discuss everything in detail.
- Please try to enable the models to H2A and other models to be able to talk to each other, such that the GREET model is not updated by hand, as shown in the presentation.
- Please delineate all assumptions and methods in documentation attending the model, especially significant assumptions regarding vehicle efficiency.
- Because researchers disagree about the relative efficiency of fuel cell vehicles and internal combustion engine vehicles (and their hybrids), please very carefully outline all assumptions and literature sources and modeling methods behind slide 10.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.5** based on accomplishments.

- The results this year are instructive, relating to the importance of government forcing (incentive) to start the vehicle fleet that allows manufacturers to bring down FCV costs.
- The most interesting result to me – though it was only mentioned briefly in the presentation – is the unstable equilibrium that can occur in the transition; if vehicle costs don't meet targets, then even a government kick-start of an initial fleet cannot produce a sustainable market for the vehicles. We have witnessed this phenomenon in other alternative vehicle programs (natural gas, battery-electric).
- Significant progress has been demonstrated in using the model to examine a broad range of scenarios and sensitivities to highlight key issues and results.
- Main barrier is to get validation of the results. I don't see where you address this.
- One interesting results is shown in Slide 12, which is that even if all the technical and cost goals for fuel cell vehicles are met, their market penetration would be essentially non-existent to 2050.
- Another interesting result is that a \$25/ton of CO_2 carbon tax results in CO_2 emissions being reduced by more than half, whereas without the carbon tax, even with fuel cell vehicles, there is no reduction in carbon emissions.
- What is the degree of confidence in these results? If high, the entire DOE hydrogen program needs to revisit its assumptions and targets, at the very least.
- Combining the various existing models and codes along with collecting much new information to yield numerous additional inputs and arrive at coherent (if not completely believable) results represents an impressive accomplishment.
- Please add greater Monte Carlo capability – a distribution of inputs (such as fuel cell vehicle efficiency) that result in a distribution of results (not single values).
- Please enable users to change parameters, such as natural gas reforming efficiency, because the technology performance changes and this has implications for the results.
- Please enable the model to be changed according to an individual company's technical progress. For example, a developer of a new wind turbine design should be able to plug their design parameters (such as capacity factor) into the model to gauge the difference between their technology and the baseline technology assumed in the model.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.5** for technology transfer and collaboration.

- The authors transfer their results to the community, but there does not seem to be a clear path to sharing the model, or implementing it into other efforts, such as the MSM.
- The project has appropriate partners.
- Peer review step is important and a good step.
- Excellent use of existing models and databases. The project team works well with other model developers and analysts.
- The project has good collaborations with other national laboratories, universities, and industry.
- Collaboration among the participating partners seems to be excellent, but for this type project, open information to the groups who could actually use it is very important.
- Please publicize GREET workshops more widely.
- Please actively work with other DOE model developers to reconcile inconsistent assumptions and methods between GREET and other DOE models.
- Please use the model to make at least one very high impact publication that is very visible (such as Science or Nature). This will also help advertise the model.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.5** for proposed future work.

- The project as described seems to be nearing a completion, except to follow other model updates and participate in international studies.
- Specific objectives are defined for FY 08.
- Future work is based on updating the model with H2A changes and other data source improvements. Vehicle technology characterization will be expanded to include plug-in hybrids and plug-in fuel cell vehicles.
- Will publish model documentation and results from analyses.
- Will develop rigorous representation of uncertainties.
- Will update and incorporate additional technology options.
- Will participate in transition analyses by the IPHE (International Partnership for the Hydrogen Economy).
- The proposed activities to the completion of this project seem appropriate.
- There was no mention of any type of follow-on or project extension.
- The future of this model should be enabling users to have more control over input parameters (such as efficiencies, emission factors etc).

Strengths and weaknesses

Strengths
- The model's approach is unique, and its ability to provide intuition into transition questions is very interesting.
- Looking at some realistic transition strategies to enable the rollout of hydrogen. HYTRANS presents some realistic challenges and provides some realistic approaches to foster the rollout.
- Shows the role of policy factors above and beyond simply meeting the technical performance and cost targets.
- A collaboration effort involving combining many models and computer codes to get common results.
- It appears to be a well-organized and well-executed project.
- The PI has done a tremendous job gathering tons of controversial technical, environmental, and other data to build this model and update it.
- The PI deserves recognition for making the GREET model in such detail and making it an industry standard.

Weaknesses
- The output is only as good as the assumptions that are input. It appears as if small changes to input assumptions can make for large result variations. The result is that there is substantial risk for early adopters who rely on the underlying assumptions.
- The conclusion that FCV introduction drive oil use to zero (Slide 14) does not appear realistic.
- The approach leads to results which may have little importance, as presented.
- Some important elements of the effort appear to be unavailable to non- team members.

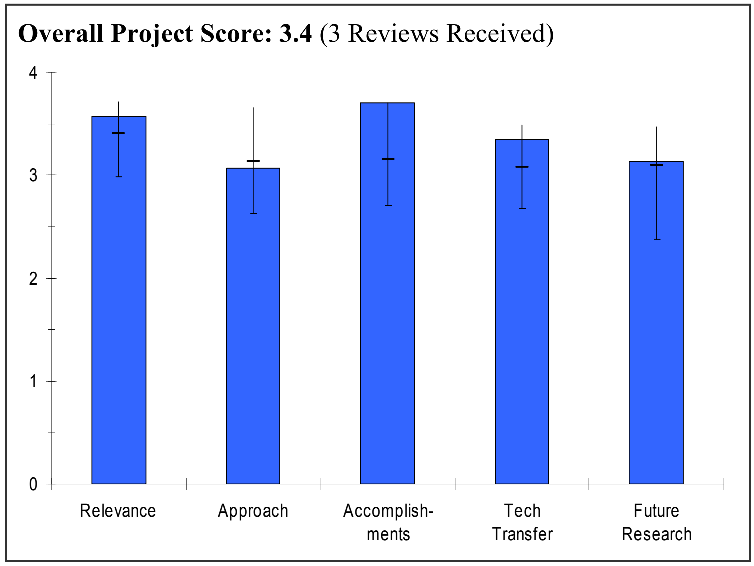
- Greater user control over input parameters is needed.
- Greater automation among GREET and other models is needed.

Specific recommendations and additions or deletions to the work scope

- Compare assumptions going forward with assumptions in previous years to consider how realistic they might be.
- Validate progress annually.
- Make sensitivity analyses a bigger part of the current study or have a follow-on study emphasizing sensitivity.
- The DOE should fund some external researchers from ANL to carefully review, critique, and possibly debug GREET, and to identify areas where the GREET model is not consistent in its assumptions and methods compared with other DOE models.

Project # ANP-01: Impact of Renewables on Hydrogen Transition Analysis
Stephen Lasher; TIAX

Brief Summary of Project



The overall objective of this project is to predict the most economically attractive renewable resources for producing hydrogen for future light-duty vehicles in the U.S. Objectives for 2006 and 2007 included 1) identify and down-select the most attractive renewable resources available in the U.S. (Lower 48); 2) establish future H_2 light-duty vehicle demand scenarios; 3) develop logistics model to minimize the delivered cost of H2 by selecting the most economical resources; 4) determine how competitive renewable-based H_2 options could be compared to fossil fuel-based (i.e. natural gas) production; 5) find what technical or cost improvements are needed to make renewable-based H_2 more competitive using sensitivity analysis; and 6) investigate H_2 delivery cost reductions by creating a pipeline network from the output of the logistics model.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.6** for its relevance to DOE objectives.

- Very valuable study to assist in understanding where priorities should be placed to enable hydrogen production from renewable resources.
- The need to understand how renewable fuels can support our overall effort is very important.
- The project is highly relevant to understanding the cost of producing hydrogen from renewable resources.

Question 2: Approach to performing the research and development

This project was rated **3.1** on its approach.

- This model does not include realistic market forces, such as competition for resources.
- Approach appears to be constrained by limited funding.
- The approach is based on realistic GIS information on hydrogen demand and renewable resource distributions.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.7** based on accomplishments.

- Excellent results (within the limits of the study) showing quasi-optimal solutions.
- Finished on time, what more can you say.
- A tremendous amount of technical results and insights, considering the minimal project time (5 months) and funding ($100K).

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.4** for technology transfer and collaboration.

- TIAX has done an excellent job of utilizing prior studies as input for this study.
- Although there has been interaction with NREL, it would have been good to have more interaction directly with the EERE offices of Wind, Solar and Biomass.
- PI should consider having direct industrial partner to get better technical inputs than the NHA working group.
- Good interaction and review of results with NREL and NHA.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.1** for proposed future work.

- If this project is continued, the proposed list of future activities is good and represents many of the things that must be done.
- If this is continued, competition for biomass resources, electricity for the grid rather than electrolysis of H_2, etc. should be included.
- It would be good to put more emphasis on identifying the barriers to achieving low cost hydrogen from renewable resources.
- Program ended but future research is very good.
- Although the project is 100% complete, the work should be extended further. A good set of further model enhancements and further sensitivity studies have been proposed.

Strengths and weaknesses

Strengths
- Excellent analysis on probable cost of producing and distributing renewable hydrogen.

Weaknesses
- Could have done a better job on identifying and prioritizing specific barriers that would lead to economical renewable hydrogen.
- Does not factor in competition for biomass resources and the option/competition to sell electricity to the grid.
- Does not include an economic trade off analysis of pumping hydrogen through a pipeline vs. sending electrons through the grid and performing distributed electrolysis.
- PI needs to have more direct industry collaboration. Cost per kg seemed optimistic, where are the taxes? For a prediction in 2030 or 2050 timeline, there will be taxes on these fuels.

Specific recommendations and additions or deletions to the work scope

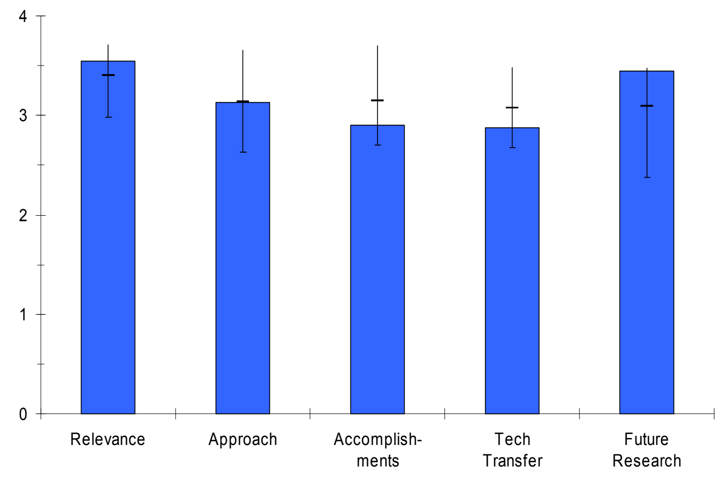
- Project is completed; however, if it is continued, the list of recommended extensions plus the addition of competing market forces should be considered.
- The model should be validated.
- PI needs to consider real world factors when you are projecting out to 2030 or 2050, cost of natural gas, cost of resources, investment cost, etc.

Project # ANP-02: Hydrogen Analysis: H2A Update 2007
Todd Ramsden; NREL

Brief Summary of Project

The H2A model aims to make analyses consistent, transparent, and comparable. Phase II goals are to reflect current DOE program direction, reflect best understanding of available technologies (including cost assumptions and performance assumptions), simplify the model structure and the user interface, improve transparency, and provide new features. New features include plant size scaling, automated sensitivity analyses and graphing, carbon sequestration costs and amounts, well-to-wheel and well-to-pump emissions calculations, and a toggle for using Annual Energy Outlook 2007 prices. The model is meant to be a means of reporting assumptions as well as calculating minimum hydrogen selling price.

Overall Project Score: 3.2 (4 Reviews Received)



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.6** for its relevance to DOE objectives.

- Understanding the cost for producing hydrogen through each pathway is absolutely essential.
- No question hydrogen infrastructure is critical to the overall market of fuel cell products, especially automotive.
- Since many of the other analysis models use outputs from H2A production, getting H2A production costs right is highly relevant.
- The project is worthwhile in that it could inform corporate and DOE decision making. My sense, through, is that this is not a model that is widely needed since it leaves out a few key issues, both political and economic.

Question 2: Approach to performing the research and development

This project was rated **3.1** on its approach.

- Financial parameters are very realistic for our economy today, but should be reconsidered annually to assure they remain realistic.
- The planned approach of taking GREET WTW/WTP results and placing them in the model as lookup tables could lead to potential errors if the tables are not rerun regularly.
- In this development, did PI leverage existing/previous work done in this field (i.e. IHIG)?
- This is a generally effective route to decision making in a flat world – one where every kg of hydrogen is worth the same.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.9** based on accomplishments.

- Progress made considering funding and time constraints is very good.
- Some assumptions cannot be correct such as 100% equity and $5000/acre. This is not realistic of the market across the nation.
- Progress looks good, but there is no benchmark or relevant measure of the extent to which some goal is being achieved.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.9** for technology transfer and collaboration.

- Solid team developing the model.
- Availability of the model needs to be more widely disseminated.
- The project needs collaborators (Air Gas, Air Liquide, etc) who are in this business to give credibility to the model.
- Available on the internet – could be better advertised.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.5** for proposed future work.

- Expanding the model to include the cost impact of hydrogen quality should draw on the ANL project, "Hydrogen Quality Issues for Fuel Cell Vehicles".
- Water use and water quality must be added to the model and should be given very high priority.
- Proposed future work sounds good and is quite relevant. However, without some sort of industrial partner in the business, it is uncertain how this work will be valued to the community.
- Adding the impact of hydrogen fuel purity on production costs is important, and could alter the relative costs for different pathways.
- Proposals seem reasonable – add in transport costs review other fuels and signs. More could be added in – see recommendations.

Strengths and weaknesses

Strengths
- Excellent start on an economic model of the production of hydrogen.
- Did not cost much – potentially quite useful.
- Transparent. Available world wide via the web.

Weaknesses
- There seems to be a tendency to make this a stand alone model, rather than one that incorporates other models (i.e. GREET) and draws on them to make appropriate calculations.
- Not clear how this model is better than previous model developed by other groups. Lack of gas supply industrial partners.
- The world is not flat – the customer has been left out of the picture to an extreme degree. Units are not readily understandable. Outputs are far too large. I don't believe that advanced nuclear should be directly compared to electrolysis – the risks are far different.

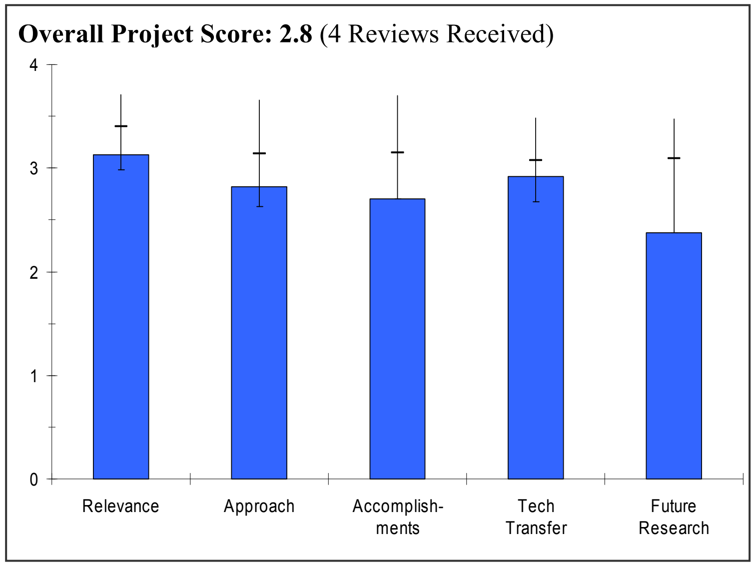
Specific recommendations and additions or deletions to the work scope

- Validation of the model must be added to the future plans.
- Incorporate GREET, H2 Quality model, etc. into this one, rather than try to duplicate their function.
- Incorporate the cost of safety when realistic information becomes available.
- PI need to gather the support of a large gas supply partner who knows the business.
- Include some estimate of transport and compression costs, include storage
- Include a basic treatment of scalability – today's fueling stations need 100 kg/day if that much. Include realistic equipment life and decommissioning. Use units people are familiar with – $/MM BTU, $/gal, $/ton of steel.

Project # ANP-03: System Dynamics: HyDIVE – Hydrogen Dynamic Infrastructure and Vehicle Evolution Model
Cory Welch; NREL

Brief Summary of Project

The objectives of this project are to 1) quantify and better characterize the nature of the "chicken-and-egg" barrier of hydrogen stations and hydrogen vehicle demand, and 2) identify high leverage strategies and policies for the development of the hydrogen transportation market through spatial, temporal simulation. HyDIVE is a dynamic, spatial, and behavioral market simulation model. System behavior results from decision-making processes of individuals. Vehicle choice model parameters are quantified via discrete choice analysis.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.1** for its relevance to DOE objectives.

- Understanding the market penetration rate of these technologies is relevant to the initiative and extremely important.
- Consumer acceptance should NOT be a DOE RD&D objective.
- Government has no role or responsibility for marketing when that is best done by the private sector.

Question 2: Approach to performing the research and development

This project was rated **2.8** on its approach.

- Appears to have significant overlap with project AN-3, by George Tolley.
- Surveying consumers regarding "alternative fuels" may not result in accurate information regarding their attitude toward hydrogen.
- Excellent approach to evaluation of the introduction of generic alternative fuels.
- Not clear what the technical barriers were.
- The PI did not identify the chicken/egg situation of whether hydrogen infrastructure/fuel cell vehicle, but this is NOT a technical barrier. It is an economic barrier, thus, out of scope.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.7** based on accomplishments.

- Analysis of consumer response to refueling station density is very good.
- Detailed assessment of 400 and 750 station cases is very good, providing useful views within two slices of time.
- Tornado chart is very good for providing quick look at where the high sensitivities are.
- While the PI seems to be touting progress and meeting milestone schedule, the accomplishments are inconsequential.
- The PI said that the research concluded that we really have a chicken/egg problem. This conclusion does not solve the problem.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.9** for technology transfer and collaboration.

- Long list of partners, but their contributions appear to be very limited.
- The research fails to consider lessons learned from the introduction of other alternative fuel vehicles.
- The research fails to examine how the chicken/egg situation was addressed with the introduction of the automobile.
- Did we have gas stations first or automobiles first?
- The research also failed to collaborate with the PI for AN-3, which is a similar research project.
- Great broad collaboration.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.4** for proposed future work.

- The proposed addition of a more vigorous modeling of the vehicle availability dynamics is very good, but there is much more that needs to be added and some things, such as perceived safety may be more important.
- No plans for future research.
- Should integrate results with RCF behavioral model to see how they correlate.

Strengths and weaknesses

Strengths
- Within the limits of the accuracy of the assumptions, this project will help understand the number of refueling sites required for sustainable growth.
- This model may already be used by the Biomass Program, but if it is not it should be.
- Sound behavior analysis based on evidence – not empirical.

Weaknesses
- Actual projections may not be realistic for hydrogen due to consumer safety perceptions and other concerns beyond station location convenience.
- Research project did not solve the problem it started out to solve; it merely went through a series of analyses only to confirm that there is a real chicken/egg problem with hydrogen infrastructure/fuel cell vehicles.

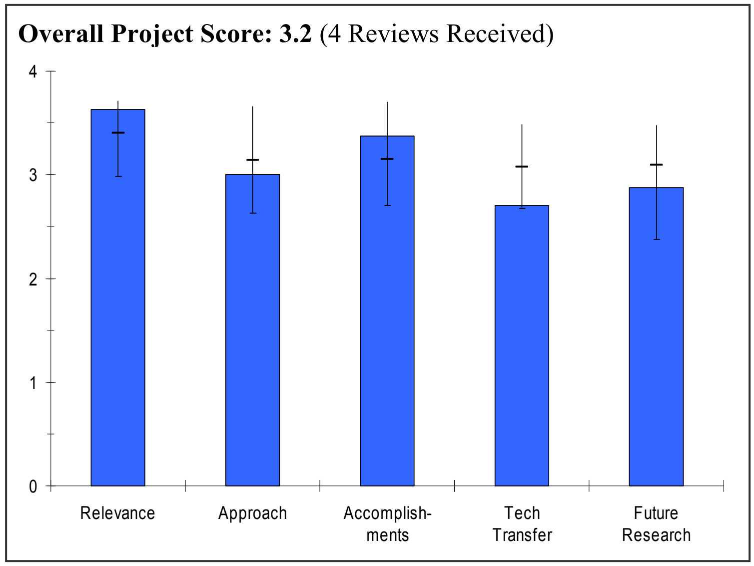
Specific recommendations and additions or deletions to the work scope

- Consumer concerns regarding safety, including safety perceptions, refueling concerns, etc. should be included to get a more accurate assessment of what will be required to achieve sustainable growth.
- Information regarding the plans for validation should be included in any future activity.
- Consideration should be given to combining this activity with the Agent Based Modeling activity to establish complimentary tasking rather than what appears to be overlapping tasking.
- No further funding of market research is recommended.
- DOE should NOT fund any research projects involving analytical models in which the model cannot be validated or collaborated.
- Need to line experimental-based behavioral models to non experimental-based.

Project # ANP-05: Analysis Repository
Melissa Lott; ATS

Brief Summary of Project

The objectives of this project are to 1) create a searchable online database of hydrogen-related analyses; 2) populate the database with as many hydrogen-related analyses as practical, both DOE- and non-DOE-funded; and 3) develop a user-friendly interface that provides the needed functionality, particularly regarding search capabilities. A library-card index approach is employed: each entry in the repository will contain enough information on the analysis or model to identify its general purpose and scope and enable the user to locate further information.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.6** for its relevance to DOE objectives.

- A single source for relevant H_2 analysis results will be very beneficial for the initiative and when reasonably populated, will save researchers time.
- Project promises to provide a "one-stop shop" or clearing house (by means of a web site) for H_2 analyses and models. This objective makes sense, and is probably long overdue.
- A central clearinghouse or repository of data on analysis and analytical models would be needed even if it were not listed explicitly as a DOE RD&D objective.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- Voluntary submission of information is frustratingly slow and frequently incomplete.
- The technology and approach used (web sites) is well understood and relatively low risk.
- The biggest risk to this project is lack of response from model & analysis owners and authors, which the project performers will try to mitigate by personally adding entries for projects for which there is no responding POC.
- Not clear how data on non-DOE sponsored analysis and analytical models will be captured.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.4** based on accomplishments.

- The repository gives ready access to 75 analyses.
- The web site is up and running and already has 75 entries. Response rate from model developers and analysts is good, per presenter.
- The repository is up and running with 75 analyses or analytical models already included and accessible to the public.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.7** for technology transfer and collaboration.

- Data is available to all – outstanding technology transfer.
- Collaboration within the Program is also outstanding and this team is getting great input, considering it is all voluntary.
- The project is all about technology transfer & collaboration, in particular with making researchers and analysts aware of model development & analyses that has already been done.
- PI did not evince collaboration with industry, universities, or other organization that have similar repositories.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.9** for proposed future work.

- Expanding the database and asking other analysts for feedback on its functionality are natural next steps.
- Plans are straightforward – advertise web site to model owners and analysts, fill out entries for more projects, add search capabilities (keyword) to allow users to more quickly navigate through the project entries/descriptions on the web site.
- See recommendations below.

Strengths and weaknesses

Strengths
- Single location for researchers to quickly search on prior work to reduce/avoid duplication.
- Low cost.
- Low risk.
- If researchers/analysts/model owners use the web site, will potentially save time.
- The repository collects data on analysis and analytical models even if not funded by DOE.
- Much needed central database for all HFCIT related projects.

Weaknesses
- Strictly dependent on voluntary submission of information; therefore, very likely to remain incomplete.
- Will not result in breakthroughs in technology or analysis. Payoff will be in time savings of other researchers, which may not be easy to measure.
- Not clear how the repository endeavors to collect data on analysis and analytical models NOT funded by DOE.

Specific recommendations and additions or deletions to the work scope

- Brainstorming session on how to create incentives for analysts to supply information.
- Has a request for analysis project information been submitted through IPHE? If not, might be worth a short presentation at the next IPHE meeting.
- Consider coordinating with other hydrogen research programs, e.g. those led by EU, to save on duplication of effort in cataloguing projects.
- Need a strategy for collecting data on analysis and analytical models NOT funded by DOE.
- Engage NE, FE, and BES early to get their buy-in and participation.

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Appendix B

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PD-6	Zeolite Membrane Reactor for Water-Gas-Shift Reaction for Hydrogen Production	Jerry Y.S. Lin	Arizona State U
SA-5	Hydrogen Release Behaviour	Chris Moen	SNL
ST-11	Hydrogen Storage Materials with Binding Intermediate Between Chemisorption and Physisorption	Juergan Eckert	UC-Santa Barbara
ST-12	Discovery of Novel Complex Metal Hydrides for Hydrogen Storage through Molecular Modeling and Combinatorial Methods	Greg Lewis	UOP
ST-13	Complex Hydride Compounds with Enhanced Hydrogen Storage Capacity	Susanne Opalka	United Tech. Res. Center
ST-19	Transition Borohydride Complexes	Craig Jensen	Univ. of Hawaii
ST-33	International Standardized Testing Protocols for Hydrogen Storage Materials	Karl Gross	NREL/HyEnergy
FC-24	Dimensionally Stable High Performance Membrane	Han Liu	Giner Inc.
BES-1	Transport Phenomena and Interfacial Kinetics in Planar Microfluidic Membraneless Fuel Cells	Hector Abruna	Cornell University
BES-2	The Development of Nano-Composite Electrodes for Natural Gas-Assisted Steam Electrolysis for Hydrogen Production	Raymond Gorte	University of Pennsylvania
BES-3	Nanocomposite Proton Conductors	Lutgard De Jonghe	Lawrence Berkeley Nat. Lab.
BES-4	Proton Exchange Membranes for Next Generation Fuel Cells	Joseph DeSimone	U of North Carolina at Chapel Hill
BES-5	Water Nanochannels in Nafion: Quantitative Scattering Analysis and NMR	Klaus Schmidt-Rohr	Iowa State University
BES-6	Charge Transfer, Transport, and Reactivity in Complex Molecular Environments: Theoretical Studies for the Hydrogen Fuel Initiative	Michel Dupuis	Pacific Northwest Nat. Lab.
BES-7	Polymer Functionalized Zeolite Proton Exchange Membrane (PFZ-PEM) for Medium Temperature (>120oC) Fuel Cells from Theory, Simulation, and Experiment	William Goddard, III	California Inst. of Tech.
BES-8	Computer Simulation of Proton Transport in Fuel Cell Membranes	Gregory Voth	University of Utah
BES-9	Porous and Glued Langmuir-Blodgett Membranes	Steven Regen	Lehigh University
BES-10	Nanostructured, Metal-Ion Modified Ceria and Zirconia Oxidation Catalysts	Maria Flytzani-Stephanopoulos	Tufts University
BES-11	Nanostructured Metal Carbide Catalysts for the Hydrogen Economy	Ram Seshadri	U of California, Santa Barbara

BES-12	Development and Mechanistic Characterization of Alloy Fuel Cell Catalysts	Anders Nilsson	Stanford Linear Accelerator Center
BES-13	Atomic-scale Design of a New Class of Alloy Catalysts for Reactions Involving Hydrogen: A Theoretical and Experimental Approach	Manos Mavrikakis	University of Wisconsin-Madison
BES-14	Metal and Metal Oxide-Supported Platinum Monolayer Electrocatalysts for Oxygen Reduction	Radoslav Adzic	Brookhaven National Lab.
BES-15	Strategies for Probing Nanometer-Scale Electrocatalysts: From Single Particles to Catalyst-Membrane Architectures	Carol Korzeniewski	Texas Tech University
BES-16	Reactivity and Stability of Multimetallic Nanocatalysts in Acid Medium	Perla Balbuena	Texas A&M University
BES-17	Studies of Model Electrocatalysts for Fuel-Cell Cathodes	Hoydoo You	Argonne National Laboratory
BES-18	High Performance Nano-Crystalline Oxide Fuel Cell Materials: Defects, Structures, Interfaces, Transport, and Electrochemistry	Scott Barnett	Northwestern University
PDP-3	Montana Palladium Research Initiative/Biological Production and Separations	John Peters	Montana State University
PDP-4	Photobiological Hydrogen Research at FIU	George Philippidis	Florida International University
PDP-7	Distributed Bio-Oil Reforming	Bob Evans	NREL
PDP-12	Low-Cost, High-Pressure Hydrogen Generator	Cecelia Cropley	Giner Electrochemical
PDP-13	Cost Reduction of High-Pressure Hydrogen Generation from Electrolysis	Steve Cohen	Distributed Energy Systems
PDP-14	Development of a Novel Efficient Solid-Oxide Hybrid for Co-generation of Hydrogen and Electricity Using Nearby Resources for Local Applications	Greg Tao	Materials and Systems Research
PDP-15	High Performance Flexible Reversible Solid Oxide Fuel Cell	Jie Guan	GE HPGS
PDP-18	Materials Solutions for Hydrogen Delivery in Pipelines	Muralidharan Govindarajan	ORNL
PDP-20	Solar-thermal Mn2O3/MnO Thermochemical Cycle to Split Water	Todd Francis	U of Colorado
PDP-21	Robust Low-Cost Water Gas Shift Membrane Reactor for High-Purity	Mark Fokema	Aspen Products Group
PDP-22	Production and Storage of Hydrogen Using C1 Chemistry	Gerald Huffman	U of Kentucky Consortium
PDP-24	UNLV High Temperature Heat Exchanger Development	Tony Hechanova	UNLV
PDP-25	Membrane Applications for Nuclear Hydrogen Production Processes	Brian Bischoff	ORNL
PDP-27	Modeling and Diagnostics of HTE Components	Bilge Yildiz	ANL
PDP-29	HyPEP Model Development	Steve Sherman	INL
PDP-34	Critical Research for Cost-effective Photoelectrochemical Production of Hydrogen	Liwei Xu	Midwest Optoelectronics

PDP-35	Combinatorial Development of Water Splitting Catalysts Based on the Oxygen Evolving Complex of Photosystem II	James Allen	Arizona State U
PDP-38	GE Solar Water Splitting: Photocatalyst Materials Discovery and Systems Development	Thomas McNulty	GE Global Res.
PDP-39	Production of Hydrogen for Clean and Renewable Sources of Energy for Fuel Cell Vehicles	Xunming Deng	University of Toledo/Bowling Green
PDP-41	Production, Fuel Cell, and Delivery Research	Yogi Goswami	U of South Florida
PDP-43	Generation and Solid Oxide Fuel Cell Carbon Source Sequestration in Northwest Indiana	Paul Matthews	Acumentrics
PDP-44	Advanced Liquid H2 Production Techniques	Martin Shimko	Gas Equipment Engineering Corporation
ANP-1	Impact of Renewables on Hydrogen Transition Analysis	Stephen Lasher	TIAX
ANP-2	Hydrogen Analysis: H2A Update 2007	Todd Ramsden	NREL
ANP-3	System Dynamics: HyDIVE – Hydrogen Dynamic Infrastructure and Vehicle Evolution Model	Cory Welch	NREL
ANP-5	Analysis Repository	Melissa Lott	ATS
TVP-3	Quantifying Consumer Sensitivity to Hydrogen Refueling Station Coverage	Corey Welch	NREL
TVP-7	Power Parks System Simulation	Andy Lutz	SNL
TVP-12	Hawaii Hydrogen Center for Development and Deployment of Distributed Energy Systems	Richard Rocheleau	Hawaii Natural Energy Inst.
STP-1	Neutron Characterization in support of the Hydrogen Sorption Center of Excellence	Dan Neumann	NIST
STP-5	DOE Carbon-based Hydrogen Storage Center of Excellence Overview Poster	Lin Simpson	NREL
STP-8	Safety Analysis and Applied Research on the Use of Borane-Amines for Hydrogen Storage	Clint Lane	Northern Arizona U.
STP-9	DOE Chemical Hydrogen Storage Center of Excellence Overview Poster	Bill Tumas	LANL
STP-15	Process for the Regeneration of Sodium Borate to Sodium Borohydride	Oscar Moreno	Millenium Cell, Inc.
STP-16	Chemical Hydride Slurry for Hydrogen Production and Storage	Andrew McClaine	Safe Hydrogen, LLC
STP-18	Hydrogen Storage Research	Lee Stefanakos	U of South Florida
STP-19	University of Arkansas at Little Rock Hydrogen Storage Project	Abhijit Bhattacharyya	U of Arkansas
STP-20	Expanding Clean Energy Research and Education Program at the University of S. Carolina	James Ritter	U of South Carolina
STP-22	Purdue Hydrogen Technology Program	Jay Gore	Purdue University
STP-23	Center for Hydrogen Storage Research at Delaware State University	Andrew Goudy	Delaware State University
STP-30	Metal Hydride Center of Excellence Overview Poster	Lennie Klebanoff	Sandia-Livermore

STP-32	Development and Evaluation of Advanced Hydride Systems for Reversible Hydrogen Storage	Bob Bowman	Jet Propulsion Laboratory
STP-33	High Density Hydrogen Storage System Demonstration Using NaAlH4 Complex Compound Hydrides	Dan Mosher	UTRC
STP-34	Effects and Mechanisms of Mechanical Activation on Hydrogen Sorption/Desorption of Nanoscale Lithium Nitrides	Leon Shaw	U of Connecticut
STP-35	A Synergistic Approach to the Development of New Classes of Hydrogen Materials	Jeffrey Long	UC Berkeley/LBNL
STP-36	National Testing Laboratory for Solid-State Hydrogen Storage Technologies	Michael Miller	SwRI
STP-37	Advanced Solid State Hydrogen Storage System Modeling	Bruce Hardy	SRNL
STP-38	Neutron Characterization and Calphad Computations in support of the Metal Hydride Center of Excellence	Terry Udovic	NIST
BESP-1	Silane Activation by Transition Metal Catalysts for Hydrogen Storage	Mahdi Adu-Omar	Purdue University
BESP-2	Nanoscale Building Blocks for Multi-Electron Electrocatalysis	Gilbert Brown	Oak Ridge National Laboratory
BESP-3	eNMR for In-Situ Fuel Cell Catalyst Characterization	Daniel Buttry	University of Wyoming
BESP-4	Nanostructured Catalysts for Hydrogen Generation from Renewable Feedstocks	Abhaya Datye	University of New Mexico
BESP-5	Novel Intermetallic Catalysts to Enhance PEM Membrane Durability	Frank DiSalvo	Cornell University
BESP-6	Nanoporous Metal Membranes with Monolayer-Thick Precious Metal Catalyst Skins	Jonah Erlebacher	Johns Hopkins University
BESP-7	A Surface Stress Paradigm for Studying and Developing Catalyst and Storage Materials Relevant to the Hydrogen Economy	Cody Friesen	Arizona State University
BESP-8	Cathode Catalysis in Hydrogen/Oxygen Fuel Cells	Andrew Gewirth	University of Illinois at Urbana Champaign
BESP-9	Hydrogen Storage Materials with Binding Intermediate Between Physisorption and Chemisorption	Gregory Kubas	Los Alamos National Lab
BESP-10	Novel Reforming Catalysts	Lisa Pfefferle	Yale University
BESP-11	Instability of Noble Metal Catalysts in Proton Exchange Membrane Fuel Cells: Experiments and Theory	Yang Shao-horn	MIT
BESP-12	Nanostructured Catalysts for Fuel Cells	Shane Street	The University of Alabama
BESP-13	Dehydrogenation of Boron Nanostructures	Michael Trenary	University of Illinois at Chicago
BESP-14	Multiscale Tailoring of Highly Active and Stable Nanocomposite Catalysts for the Production of Clean Hydrogen Streams	Gotz Veser	University of Pittsburgh
BESP-15	An Integrated Approach Toward Rational Nanocatalyst Design For Hydrogen Production	Dionisios Vlachos	University of Delaware

BESP-16	The Reactivity and Structural Dynamics of Supported Metal Nanoclusters Using Electron Microscopy, in situ X-Ray Spectroscopy, Electronic Structure Theories, and Molecular Dynamics Simulations	Judith Yang	University of Pittsburgh
BESP-17	Sol-Gel Based Polybenzimidazole Membranes for Hydrogen Pumping Devices	Brian Benicwicz	Rensselaer Polytechnic Institute
BESP-18	New Proton-Conducting Fluoropolymer Electrolytes for PEM Fuel Cells	Stephen Creager	Clemson University
BESP-19	Hydrogen Purification Using Advanced Polymeric Membranes	Benny Freeman	University of Texas at Austin
BESP-20	Carbon Nanotube Materials for Substrate Enhanced Control of Catalytic Activity	Michael Heben	National Renewable Energy Laboratory
BESP-21	Surface-Initiated Ionomer Films Based on Modified Poly(n-alkylnorbornene)s	G. Kane Jennings	Vanderbilt University
BESP-22	A Unified Computational, Theoretical and Experimental Investigation of Proton Transport through the Electrode/Electrolyte Interface of Proton Exchange Membrane Fuel Cell Systems	David Keffer	The University of Tennessee
BESP-23	Fundamentals of Hydroxide Conducting Systems for Fuel Cells and Electrolyzers	Bryan Pivovar	Los Alamos Nat. Lab.
BESP-24	Ab Initio Screening of Ternary Alloys for Hydrogen Purification	David Sholl	Carnegie Mellon University
BESP-25	Electrostatically Self-assembled Amphiplexes	Helmut Strey	Stony Brook University
BESP-26	Theory, Modeling, and Simulation of Ion Transport in Ionomer Membranes	Philip Taylor	Case Western Reserve University
BESP-27	Preparation of Composite Fuel Cell Membranes Containing Electric Field Aligned Inorganic Particles	Matthew Yates	University of Rochester
FCP-2	Montana Palladium Research Initiative/Catalyst Degradation	Stuart Snyder	Montana State University
FCP-3	Fuel Cell Testing at the Argonne Fuel Cell Test Facility	Ira Bloom	ANL
FCP-5	PEM Fuel Cell Freeze Durability and Cold Start Project	Mike Perry	UTC Power
FCP-6	Complex Coolant Fluid for PEM Fuel Cell Systems	Satish Mohapatra	Advanced Fluids Tech.
FCP-7	Combinatorial Screening of Fuel Cell Catalysts	Keith Kepler	Farasis Energy
FCP-10	Next Generation Bipolar Plates for Automotive PEM Fuel Cells	Orest Andrianowycz	GrafTech International, Ltd.
FCP-11	Nitrided Metallic Bipolar Plates	Peter Tortorelli	ORNL
FCP-12	International Stationary Fuel Cell System Demonstration	John Vogel	Plug Power Inc.
FCP-13	Intergovernmental Stationary Fuel Cell System Demonstration	Michael Parsons	Plug Power Inc.
FCP-14	Low Cost, Durable Seal	Jason Parsons	UTC Fuel Cells
FCP-15	Effects of Impurities on Fuel Cell Performance and Durability	Trent Molter	University of CT

FCP-16	Effects of Impurities on Fuel Cell Performance and Durability	James Goodwin	Clemson University
FCP-17	Effects of Impurities on Fuel Cell Performance and Durability	Fernando Garzon	LANL
FCP-18	Adaptive Stack with Subdivided Cells for improved stability, reliability, and durability under automotive load cycle	Bin Du	Plug Power Inc.
FCP-19	Light-weight Low-cost PEM Fuel Cell Stacks	Jesse Wainright	Case Western R Univ
FCP-20	Low-Cost Manufacturable Microchannel Systems for Passive PEM Water Management	Ward TeGrotenhuis	PNNL
FCP-21	Subfreezing Start/Stop Protocol for an Advanced Metallic Open-Flowfield Fuel Cell Stack	James Cross	Nuvera Fuel Cells
FCP-22	Visualization of Fuel Cell Water Trasport and Performance Characterization under Freezing Conditions	Satish Kandlikar	Rochester Institute of Technology
FCP-23	Water Transport in PEM Fuel Cells: Advanced Modeling, Material Selection, Testing, and Design Optimization.	Vernon Cole	CFD Research Corp
FCP-24	Water Transport Within the Stack: Water Transport Exploratory Studies	Rod Borup	LANL
FCP-25	Advanced Cathode Catalysts and Supports for PEM Fuel Cells	Mark Debe	3M Company
FCP-26	Highly Dispersed Alloy Cathode Catalyst for Durability	Tom Jarvi	UTC Fuel Cells
FCP-27	Advanced Cathode Catalysts	Piotr Zelenay	LANL
FCP-28	Non-Platinum Bimetallic Cathode Electrocatalysts	Debbie Myers	ANL
FCP-29	Development of Alternative and Durable High Performance Cathode Supports for PEM Fuel Cells	Yong Wang	PNNL
FCP-30	Novel PEMFC Stack Using Patterned Aligned Carbon Nanotubes as Electrodes in MEA	Di-Jia Liu	ANL
FCP-31	Improved, Low-Cost, Durable Fuel Cell Membranes	Scott Gaboury	Arkema
FCP-32	Membranes and MEA's for Dry, Hot Operating Conditions	Steven Hamrock	3M
FCP-33	New Polyelectrolyte Materials for High Temperature Fuel Cells	John Kerr	LBNL
FCP-34	New Generation High Efficiency 2 kW Fuel Cell Stationary Fuel Cell System	Durai Swamy	Intelligent Energy
FCP-36	DMFC Prototype Demonstration for Comsumer Electronic Applications	Robert Sievers	MTI Micro Fuel Cells
FCP-37	Low-cost Co-production of Hydrogen and Electricity	Jim McElroy	Bloom Energy Corp.
SAP-1	Codes and Standards	Gary Nakarado	Regulatory Logic
SAP-3	IEA Demonstration Analysis	Susan Schoenung	Longitude 122 West
STP-8	Electron-Charged Graphite-Based Hydrogen Storage Material	Chinbay Fan	Gas Technology Institute
STP-9	Nanostructured Activated Carbon for Hydrogen Storage	Israel Cabasso	State University of New York

STP-18	Advanced Concepts for Containment of Hydrogen and Hydrogen Storage Materials	Andrew Weisberg	LLNL
EDP-1	Hydrogen Knowledge Survey	Tykey Truett	ORNL
STP-37	Hydrogen Storage in Novel Organic Clathrates	Peter McGrail	PNNL
TVP-6	Novel Compression and Fueling Apparatus to Meet Hydrogen Vehicle Range Requirements	Todd Carlson	Air Products
TVP-9	Detroit Commuter Hydrogen Project	Carmine Palombo	SEMCOG
EDP-1	Code Official Education	Lynnae Boyd	NREL
STP-21	A Cassette Based System for Hydrogen Storage and Delivery	Wayne Britton	FST Energy
FCP-35	DMFC Power Supply for All-Day True-Wireless Mobile Computing	Brian Wells	Polyfuel, Inc.

APPENDIX C: FY 2007 MERIT REVIEW AND PEER EVALUATION MEETING: FEEDBACK AND RECOMMENDATIONS

These notes summarize the comments received from various participants at the May 15-18, 2007 Review:

Section 1: Comments received from Peer Reviewers during feedback sessions held immediately after each subprogram track was completed. The comments received were generally focused on the basic review process; however, where relevant, notes specific to a particular subprogram session are included.

Section 2: Scores and summarized answers to questions from the Review Questionnaire, filled out by approximately 61 of the participants.

Section 1 – Peer Reviewer Comments

General Review Comments

- The presenters did a good job.
- A few more minutes for the presentations would be good. Maybe 10 minutes more to cover more material - especially for those with media (videos and radio) - since those are the products we are evaluating.
- Suggestion: Have presenters share when and where products are/will be available.
- Twenty minutes is not enough time for many of the presentations the way they are given. Either thirty minutes needs to be allotted for each presentation, or keep the length at twenty minutes and force the presenters to focus on the point.
- Many of the presenters need to be taught how to present.
- Reviewers felt that they had been given early enough access to the presentations online before the week of the Annual Merit Review.
- Why are some projects presented as posters instead of oral presentations? It was explained that new projects that started only a few months ago are presented as posters.
- Suggestion: The Reviewer selection and assignment process should include having potential Reviewers check-off their areas of expertise as they pertain to the AMR, so that Reviewers will receive more appropriate project assignments.
- There needs to be some sort of attendance confirmation for the very last talks of the Review.
- The Kick-Off Meeting is redundant.
- Suggestion: Either shorten the poster sessions or hold them all on one to two nights.
- There were not enough guest rooms available at the hotel. Suggestion: Registrants must pre-pay for the hotel room when they register to help prevent people from backing out of attending at the last-minute, thereby minimizing disruptions to the review assignments.
- The Safety, Codes and Standards information in the Plenary Sessions was not of pertinence to everyone. However, other Reviewers disagree with this statement and feel that it is a useful and justified overview.
- Sessions ran on schedule and there was plenty of time for questions.
- Conflict in the timing of sessions of the three tracks made it difficult for participants to attend sessions in different tracks.

- May extend number of conference days next year or only review 50% of the program.
- Next conference to be held in June 2008. Many researchers attend 3 other meetings held around the same time so difficult to avoid conflicts.
- Reviewers should not be assigned only posters to review.
- Reviews for each reviewer should be spread out more evenly over the course of the meeting.
- Need a clear directive on the time frame for the accomplishments Reviewers are evaluating. There's uncertainty as to whether reviews should cover exclusively last year's accomplishments, or accomplishments of the project as a whole. Also, all of the speakers need to present in the same time frame – either last year or the entire project.
- It is unclear as to how much weight in the score should be given according to the work performed last year versus work performed in the entire project.
- It would be useful if general background of a project since its inception – a kind of historical perspective – was provided. This would be particularly useful for new and first time Reviewers to be able to put the project into perspective.
- It is good that foreign Reviewers are invited to participate in the Review – to keep the Review open and provide a broad perspective.
- The overall flow of the Review was improved. Fewer reviews per Reviewer was helpful.
- Comments from first year Reviewers:
- Thought the Review would be chaotic; instead it was streamline.
- Compared to other Reviews attended (outside of the Hydrogen Program), this one was much smoother.
- Had a positive review experience.
- The Kickoff Meeting: There is not tremendous value in hearing the same 20-minute talk each year. Suggestion: Have the TDMs speak to their Reviewers prior to the review to provide guidelines on how the projects should be evaluated (as oppose to the mechanics of how to fill out a form). This way, the Reviewers can evaluate according to the appropriate rules they are given.

Review Forms

- The evaluation forms were good.
- There is a bit of redundancy in the forms. For example, when the Reviewer reaches the "Recommendations" section at the end of the form, he or she has already given recommendations throughout the form.
- One reviewer did not like using Excel forms.
- Reviewer questioned why "Relevance" was on Evaluation Form. Answer: This section was originally intended to compare earmarked vs. non-earmarked projects. In the future, maybe just put "yes" or "no" with explanation if answer is "no."
- The evaluation of partnering is practically pointless right now and preferably should be dropped. It is unclear why partnering is even a requirement that gets scored (people can do good work alone or within their institutional team).
- The Evaluation Forms are good for research and development type projects, but are not as well suited for Technology Validation projects. *Suggestion:* The Technology Validation evaluation forms would ideally focus more on the usefulness of the project to the public and to safety.
- Would like the opportunity to provide a subjective perspective on the value of the projects.

Education Review Session

- Reviewer Question: What kind of evaluation process is in place?
    - Facilitator Response: An evaluation process is planned and very important to our project. Preliminary deployments are being conducted and we are receiving ongoing feedback from teachers and students. As we move out into more schools, we are planning to incorporate evaluation mechanisms to aid future updates and improvements.
- Reviewer Question: Are website downloads tracked?
    - Facilitator Response: It is tracked, but not being looked at right now.
- Reviewer Question: How long does it take to train teachers?
    - Facilitator Response: Training a teacher with a good science and chemistry background can be as quick as 15 minutes. Teacher training workshops typically last 1 day but can be as short as 2 hours, depending on the time available.
- Reviewer Question: Can the teachers afford the kit on the $200 income tax deduction?
    - Facilitator Response: The kits cost $500 and have been designed for use over multiple years in multiple classrooms. Teachers who attend the workshops receive the kits free of charge.
- Reviewer Question: You seem to have covered the broad spectrum of the emergency response and hydrogen community in the review and outreach process, but as hydrogen is adopted in the widespread community, how will you deal with safety training of private security staff, university employees, etc?
    - Facilitator Response: You bring up a good point – we should begin to consider who else should be included in safety training. The course was designed to be widely accessible and we will consider how we can extend our outreach, especially in areas where demonstrations exist.
- Reviewer Suggestion: The Federal Aviation Agency has developed a system to track use of online training modules (time spent on each page, testing, other tracking mechanisms). You should consider looking at their system as a model for certifying course completion.
    - Facilitator Response: This is something we are considering for the future and we will take a look at this work.
- Reviewer Suggestion: At the EERE Info Center we get questions like, "We are putting in a hydrogen lab at a university, what do we need to know in terms of safety?" This course could fulfill the need to educate those who are installing hydrogen and fuel cell facilities by informing them about the essentials of hydrogen safety.
- Reviewer Question: Regarding the dichotomy of education, outreach, and messaging - on one hand we have all this language about how incredibly safe hydrogen is – how quickly hydrogen is dispersed, tanks are impenetrable, etc. On the other hand, we are always talking about fire fighters, emergency responders, and police in connection with hydrogen. How do we balance these two sides and ensure that the public doesn't get the wrong impression?
    - Facilitator Response: This is something we have discussed and considered extensively, in terms of how and whether to raise the issue of safety. When we are addressing the general public we try not to bring it up unless someone asks a specific question. Compared to other emergency safety training courses that include lots of sensationalistic materials – such as flames, explosions, or blood - we have taken a different approach and created something more neutral, even though the flashy design approaches are what attract the attention of firefighters. We were also very conscious with the wording of the course material and take special care to be truthful but not alarming.

- Reviewer Question: Is there a multi-year plan for how these various activities are going to contribute to the overall goals of the hydrogen program?
    - Facilitator Response: We have an MYPP for education which addresses the safety and codes target audience that is a large focus of the education activity. When collaboration with the Safety, Codes, and Standards Program Element began, we developed a high-level, multi-tiered plan to address the various education needs of this audience.
- Reviewer Question: You mentioned that there are variations in audiences across the country. Can you elaborate on this?
    - Facilitator Response: There are two components to this issue – we need to speak to different audiences in different voices but we also need to concentrate our communications where demonstrations exist and focus the message around a specific facility.
        - As an example, the first radio spot was fairly general and could be used by states where strong local initiatives for hydrogen and fuel cells have begun but facilities have not yet been installed. In contrast, the second spot is specifically about cars and will be deployed where stations and vehicle demonstrations are a visible entity in the local community.
- Reviewer Question: Will the podcasts be available for states to use and what is the process for states to incorporate them into their outreach materials?
    - Facilitator Response: We have just begun a concentrated effort to strengthen our relations and communications with state and local initiatives. As we finalize the podcasts, we will establish a protocol with our communications office to ensure that states will be able to use the podcasts and any of our other educational materials.
- Reviewer Question: Why do you emphasize how few fueling stations there are? If you start your messaging campaign with an idea of scarcity and smallness, as more and more stations are installed it will become difficult to change that messaging and change that mindset about hydrogen as a future technology.
    - Facilitator Response: We are very careful about overselling and we do not want to give anyone the impression that there will be a station somewhere where they will not see hydrogen and fuel cells for a while. We do not want to risk overselling the technology, especially on the vehicle side. As the market develops, so will our communications strategy and messaging.

- Suggestion: It would be helpful to have a special interactive review session where Reviewers can play around with some of the education products (school kits, media, online tutorials), similar to the special Analysis Reviewer session this year. They set up the various models on laptops for the reviewers to play around with and explore in depth.

Fuel Cell Review Session

- The Reviewers are forced to be too narrowly focused on the projects they are reviewing. Reviewing 12 projects is too much – there are so many other side meetings and aspects of the Review that a Reviewer reviewing so many does not have time to participate in these other areas of the Review and have time to fill out review forms. Reviewers with 6 to 7 reviews felt the work load was reasonable.
- Twelve-hour days are too long for the Review – there is no time for networking. *Suggestion:* It would be nice if, since the Review will be held for five days next year, the activities that have been held in four can be spread out to shorten the days.

- For projects ending in six months, it would be informative to still have the presentation, but is it really necessary to review such projects?
- There was too much membrane and catalyst information packed into two days.
- On reviewing membranes projects: it is difficult to review the approach of the project if the information on the project is confidential and therefore not presented. *Suggestion:* Perhaps alter the Evaluation Form for membrane projects to account for the fact that some aspects of the projects cannot be adequately reviewed.
- Why are non-precious metals catalysts NOT part of Basic Energy Sciences? That research seems more appropriate to BES.
- BES Presentations:
    - A Reviewer asked why the BES presentations were not on the Reviewer Information Website before the meeting. It was explained that the BES presentations were not on the website because they were not being reviewed. However, they are available on the CD-ROM all registered attendees receive.
    - A Reviewer noted that the BES presentations seemed to follow a different format or had a lack of uniform format. The Reviewers wondered whether the BES PI's were given a presentation template to follow.

Hydrogen Production and Delivery Review Session

- Good/outstanding projects presented.
- Presentations lacked enough technical data to review, sometimes for proprietary reasons. Sometimes data could not be accurately interpreted due to lack of information. Request/suggestion to include section on reviewer form called "data quality."
- Reviewer commented that she could not judge progress because she did not know state-of-the-art. Response: DOE has tables with current status and targets that can be provided ahead of time (for targets). Reviewer commented that slides needed to show annual progress and not report the same progress every year.
- Standardized format for presenters was useful, but need more latitude in format to provide more depth. More information came from questions at the end.
- Presenters need to clearly define paths to targets and clearly identify a critical path of how to get there.
- Did not see any "go/no go" or "off ramps" presented.
- Transition plans need to be provided. Future plans presented, but not marketing plans.
- Researchers should mention what other research is needed to advance their own – tell what problems need to be solved (i.e., materials issues).
- The print in the legends and figures in some of the presentations was too small.
- Value of the project should be indicated based on the scope of the project given the budget provided.
- Economic questions: Reports sound as if researchers are already on their way to targets; analysis should be more realistic. There is no indication of how R&D will achieve the economics they present. Institutionalization of H2A rules may help.
- Too many electrolysis projects presented.

Systems Analysis Review Session

- Good/outstanding projects presented.
- Two deployment models are not including safety as variables. Safety will be considered later and will increase capital costs.
- Consumer perception of safety will more greatly influence use of hydrogen vehicles than distances to fueling stations.
- Use of hydrogen in ICE will be used as a comparison for GHG emissions and fuel use – will be competed in some models as an option.
- Fuel purity – trying to understand trade-offs, need to understand cost model. Is there co-contamination?
- Several of the models have overlap – is there a good reason for this?
- End users need validation of models/predictions; need to make sure that H2A is on target first.
- Next steps:
    - Look at how gasoline will be reduced; refineries will have to change operations
    - Will gasoline be exported to China and India?
    - Possibility of reforming gasoline into hydrogen
- Shift to new technologies occur at 16-25% market penetration. Shift to hydrogen vehicles will not be for convenience – must be more value added (performance, "green," fuel prices).
- In the MYPP, take credit for looking at market and technology barriers and putting them into perspective.
- Examine whether it is better to have demos before or after orals.
- Introduction to Analysis was good to show how presentations would fit together.

Storage Review Session

- A list of partners is provided on the first slide of presentations, but there is no indication as to how valuable the partners are or how much interaction there was in the work. How much work contributing to the project did they share? *Suggestion:* If presenters are required to list their partners, have them overview what the partners did and, just as important, what they did for the partners. Also, this is much more appropriate for the centers to discuss and not something for the project presenters to spend time on.
- Future plans are important but are generally blown off. In some cases, they are entirely missed. In others, future plans are given about 20 seconds and are vague and uninformative. *Suggestion:* We may need to accept that hardly anyone will time their talk, so leave an extra three minutes for plans after the presenter finishes.
- Some of the back-up slides in the project presentations should have been a part of the actual presentations.
- Solid state materials should be as important as wt.% and vol.
- Presentations should provide the project's orientation to the program. A lot of presentations simply show the results; the approach to the target is also important.
- There has been a lot of progress in this area, but still need to work on ensuring that the presentations contain only the information Reviewers need to know. At times there were quite a few slides with extraneous information in a presentation that was already too long.
- If a slide is being shown that is the same as one used in the previous year(s), the presenter needs to be clear that he/she is showing a slide from before.

- The future work of some projects was given very specifically, while others were very vague. More detail on future work would be nice.
- *Suggestion:* There were a couple of presentations in which the slides each contained just one line with the point of the slide – how the project works towards the plan. This is helpful to the audience to know what the point is right away. Also a slide with just two to three lines explaining how the project supports the plan would be useful.
- The connection between the values of the project results and the program targets is not always clear. What is the novelty of this year's results? Some slides are exactly the same as last year.
- The way some results were reported was "annoying" – or at least not very useful.
- Some of the presentations, while scientifically stimulating, were a bit ambiguous/unclear in terms of the point – Reviewers only have the presentations to rely on.
- Because scientists often tend to be very success-driven, there needs to be a clear way of saying "here we are in the project," "here is where we need to be," and "here is how/if we are going to reach that point." At times, the presenters need to be more frank about where they are in their projects.
- There are some projects that need to have (or maybe show in their presentations) their relationship with the outside world.
- Center technical accomplishments should be restricted to progress toward goals. They can mention the projects that are making the progress, but they do not need to go into the technology. *Suggestion:* The Center presentations are management presentations and should be given as such. DOE should review and, if needed, help the Centers focus their presentations on management aspects.
- It is really nice having the Centers report to us in January, February, and March, and at the Merit Review in May; but a number of slides that were presented at FreedomCAR contained errors which were pointed out and then left unchanged for the Merit Review.
- In the Center of Excellence presentations, projects were described instead of the Center. Also, the Center presentations show enthusiasm, but they also show weak plans. *Suggestion:* Would like to see the coordination that takes place through the Center. Emphasis should be on collaboration between projects and evaluation criteria for projects.
- What are the Centers of Excellence decision-making criteria?

Technology Validation Review Session

- DOE targets were not emphasized in the Technology Validation presentations, nor do the Evaluation Forms capture that aspect. The presentations and Evaluation Forms should be modified to incorporate the DOE targets.
- Safety should be a required slide in all Technology Validation presentations, and tied into the Technical Targets/Goals.
- Other people, like UPS, are using fuel cells. That data would be useful to the DOE Hydrogen Program.

QUESTIONNAIRE

DEMOGRAPHIC QUESTIONS

1a. What was your role in the review?
Total responses: 61
14 Peer Reviewer (please answer questions in Sections A. and B.)
11 Presenter of a Project -- Oral or Poster (please answer questions in Sections A. and C.)
1 Presenter of Program Overview (please answer questions in Sections A. and C.)
35 Attendee, neither Reviewer nor Presenter (please answer questions in Section A. only)

1b. What is your affiliation?

0 Government agency directly sponsoring the program under review
16 National/government lab, private-sector or university researcher whose project is under review
16 In an industry directly involved in the program under review
6 In an industry with interest in the work under review
3 Government agency with interest in the work
11 National/government lab, private-sector or university researcher not being reviewed, but who has an interest in the work
5 Other (please specify, e.g., consultant, retired employee, public, etc.) ____________

A. QUESTIONS 2 THROUGH 21 FOR ALL ATTENDEES

2.	Purpose and scope of the Hydrogen Program Review were well defined.	*disagree*				*agree*		
		1	*2*	*3*	*4*	*5*		
				4.6				
3.	The plenary presentations were helpful to understanding the direction of the Hydrogen Program.	*Disagree*				*agree*		
		1	*2*	*3*	*4*	*5*		
				4.3				
4.	Sub-program overviews were helpful to understanding the research objectives.	*disagree*				*agree*		
		1	*2*	*3*	*4*	*5*		
				4.3				
5.	The quality, breadth, and depth of the following were sufficient to contribute to a well-considered review:	*disagree*				*agree*		
	a. Presentations	*1*	*2*	*3*	*4*	*5*	**4.1**	
	b. Question & Answer periods	*1*	*2*	*3*	*4*	*5*	**3.9**	
	c. Answers provided concerning programmatic questions	*1*	*2*	*3*	*4*	*5*	**3.8**	
	d. Answers provided concerning technical questions	*1*	*2*	*3*	*4*	*5*	**3.9**	
6.	Enough time was allocated for presentations.	*disagree*				*agree*		
		1	*2*	*3*	*4*	*5*		
				4.2				
7.	Time allowed for the Question & Answer period following the presentations was adequate for a rigorous exchange.	*disagree*				*agree*		
		1	*2*	*3*	*4*	*5*		
				4.0				
8.	The questions asked by reviewers were sufficiently rigorous and detailed.	*disagree*				*agree*		
		1	*2*	*3*	*4*	*5*		
				3.8				

9. There were no problems with: *disagree* *agree*
   1. Groupings of projects by technical area *1 2 3 4 5* **4.5**
   2. Proprietary data (should not be any at this Review) *1 2 3 4 5* **4.3**
   3. Quantity/level of the information presented *1 2 3 4 5* **3.9**

10. The review was conducted smoothly. *Disagree* *agree* *1 2 3 4 5* **4.5**

11. The frequency (once per year) of this formal review process for this Program is:
    59 about right
    0 too frequent
    1 not frequent enough
    0 don't know the frequency of reviews

12. Logistics and amenities were satisfactory. *Disagree* *agree* *1 2 3 4 5* **4.6**

13. The visual quality of the presentations was adequate. I was able to see all of the presentations I attended. *disagree* *agree* *1 2 3 4 5* **4.0**

14. The audio quality of the presentations was adequate. I was able to hear all the presentations I attended. *disagree* *agree* *1 2 3 4 5* **4.3**

15. The hotel accommodations were satisfactory. *disagree* *agree* *1 2 3 4 5* **4.3**

16. The information about the Review and the hotel accommodations sent to me prior to the Review was adequate. *Disagree* *agree* *1 2 3 4 5* **4.5**

17. What was the most useful part of the review process?

- The exchange of ideas from people with common interests in research. It lets the research community know if someone else is working on a similar area at least on the government-sponsored area of science.
- Detailed talks by Directors and project leaders of the centers. The poster sessions were also of high quality.
- Overview presentations
- Obtaining feedback/guidance on the direction of the project. Chance to disseminate the learning quickly to a large number of stakeholders.
- Know how research is going and how tax money has been spent worthfully.
- Gave a pretty good idea of overall program directions.
- presentations
- Oral and poster presentations.
- Peer interactions, discussions at poster session. Very helpful to review presentations before review.
- Presentational CD
- To experience all the "parts" of H2 program and how they fit together.
- Questions by reviewers.

- Seeing all of the funded projects and what others are doing.
- One-on-one communications.
- Oral presentations.
- Hearing technical progress with respect to targets. Q&A period. (I have followed the storage part.)
- Informal gatherings (e.g. lunch, breaks, and poster sessions. Presentations on disk.
- Information and progress status obtained through the review process. Interaction with other research groups.
- Getting an overview of all hydrogen storage techniques and potential problems associated with each one.
- Access to project managers and research staff during breaks. Useful to have an update on progress.
- Meeting program managers and colleagues, networking and coming up to date with the program direction and thrust.
- Seeing the progress that has been made during the past year; keeping in touch with other researchers.
- Getting a broad overview of the goals of the DOE's Hydrogen program and future agenda.
- Consistent format for presentations. Focus on results and progress toward goals. Good framing of overall program.
- Technology validation and FC part.
- Having all projects under a subtopic together.
- I can grasp the whole (concepts, materials to tech validations) information.
- Presentations/Question, answer sessions.
- Q&A after presentations were technical exchange and "brainstorming" occurred.
- The actual presentations, poster board presentations.
- Overview at start of each section.
- Keeping the posters at the hotel is a good idea. It keeps people around. However, you need larger rooms to accommodate all the attendees during the poster sessions.
- To have the presentation slides before the meetings on a CD ROM
- Basic Energy Science Session.
- Ample breaks, meals, etc. allowed plenty of time for offline discussions and info sharing.
- 1. Reviews - Technical information on project progress, etc. 2. Poster Sessions - new ideas and activities. 3. Opportunity and ability to discuss with project PI's and others present during the week.
- Get a clear picture of the progress. FC session was very informative. Technology Demonstration was the best.
- Networking and Plenary Addresses and SOME Presentations.
- 1. Direct communication with hydrogen researchers and analysts. 2. Useful information on progress of the overall program from all parts of DOE dealing with hydrogen.

18. What could have been done better?

- Some of the plenary slides had way too much information requiring small fonts.
- Earlier poster sessions - even at the expense of lecture sessions.
- Very little.
- Need to use the opportunity to have tutorial session. There are still many misunderstandings on targets vs. research work. This is an excellent forum to cross-train a diverse group.
- Extend by one day and shorten days to allow chance for better networking/informal meetings.
- The projects with poor performance or did not have chance to meet the objectives could be

removed rather funding them for multiple years.

- Some of the presentations had small fonts. Could not be seen from the back: larger fonts would have helped. More parallel sessions with a more focused theme.
- It's very important to have person asking question stand while asking question. As a presenter, I could sometimes not determine who was asking a question or where they we located.
- Presenters could have discussed figures to a greater degree, specifying units on axes.
- Preview presentation and poster on CD before coming in so that the review process is more efficient and effective.
- As a poster presenter, some reviewers just walked by, while others made a conscious effort to engage presenter in discussion to understand project.
- It's just fine.
- When presenting, I could not hear the questions. I saw that others had the same issue. The speakers were towards the audience, so presenters had a hard time hearing the questions.
- Presenters had difficulty hearing questions from the audience. Noise from refreshment area was a major problem. No one closed doors so audience could hear the presenters.
- Less formal presentations. Not all presentations needed 30 minute slots.
- Need food at morning break - granola bars, fruit. 8am to 8pm is too intense.
- I wish to commend the organizers of the review exercise. I find it an extremely useful event and a model for other programs/areas. Perhaps a wrapping-up session where project leaders would comment on the projects for success within the remaining time period.
- Graphs and letters of some presentations should be made more clear. Interaction with other research groups.
- Sound quality was poor - too much reverberation in the sound system.
- Quality of reviewers could be improved and make sure these folks don't have a bias toward certain technologies and no conflict of interest - hidden or real.
- The slide templates were better last year - many presentations got into so much detail that the purpose of the project was lost.
- I find it hard to believe that reviewers and others gain enough insight from a 20 minute presentation to adequately evaluate a project. Some program managers scheduled separate briefings to provide more detail. This was extremely helpful.
- Presentations were hard to see due to the font size used at times. A standard presentation format that would use a font size and color coordination to allow for it to be easier to read.
- Sound system was "muddy." Also people asked questions without using microphones.
- More time for presenters and for completion of review forms.
- Time for presentation was quite limited. For better understanding, it is helpful to distribute presentation files prior to the Review/ (Say a week before?)
- Minimum font sizes for presentations. Many used small fonts.
- Fewer side meetings. (I know it is hard!) Many of the slides have too much text or data and it was hard to see small text. The frequency of the review is about right, but it is getting large!
- Should not allow people to speak on their cell phones during the review - very disruptive and distracting.
- Many participants use laptop to take notes or follow the presentations, but the rooms lack electric plugs/power.
- Larger men's room - less crowding at breaks. (staggered breaks between A/B/C would have alleviated problem.
- The biggest problem is that on Friday, most attendees are gone. Suggest that you start the plenary at 8:00 and end at 9:30. Start sessions at 10:00 on Tuesday; end each day by 6pm. If you do that, all Friday presentations would be done by Thursday Evening. Consider a 6-8pm reception on Monday evening to register most people and then you would be able to start the

plenary on Tuesday at 8:00
- Side meeting in Madison room - doorknob broken. Modeling efforts (SA) should have longer time slots.
- To have also the presentation slides of BES programs.
- 1. More presentations from industry. 2. Too much confidentiality in Technology Validation.
- Should provide tables for poster sessions to hold handouts, drinks, computer monitors to show slides or videos, etc.
- Well organized.
- Better audio systems.
- Choose better projects (higher quality projects). Some of the system analysts (e.g. PTP and TIAX were NOT relevant and overly optimistic (almost to fulfill a political agenda). Battelle work, however, was very solid and realistic.
- Limited amount of time to convey extensive and complex information on many projects can be frustrating.
- Does this time and effort make a difference?

19. Overall, how satisfied are you with the review process? *1 2 3 4 5* **4.3**

20. Would you recommend this review process to others and should it be applied to other DOE programs? O *yes* **56** O *no* **0**

21. Please provide comments and recommendations on the overall review process.

- none
- Very informative re state-of-the-art and progress toward hydrogen utilization. I don't feel the H2 approach can be sold on economics, but must depend on global warming issues - this should probably be addressed more thoroughly.
- DOE is not using the opportunity to cross-train a diverse group of researchers for example, the molecular storage folks miss the practical issues facing the validation program or vice-versa.
- Perhaps reviews should see presentation prior to meeting (don't know if this is the case now). Be aware of conflicts of interest from peer reviewers e.g. competition reviewing project will not be objective.
- Accountability should be judged for continuous funding supports. The projects without delivery should be removed. 5 year guarantee policy is not in the best interest of taxpayers.
- Overall it’s a very useful review process. It would help to have more focused and smaller group. Hotel facilities were excellent. Food was good. Poster sessions should have been a little longer.
- Review of the posters was greatly enhanced by one on one discussions.
- 1. Session should be marked on the badge. 2. Select good presentation to discuss among different sessions.
- I think this review process is essential to keep the focus on whatever goals/objectives a funded project must meet. Otherwise it is easy to go in the wrong direction especially over a year's time period.
- Some members of the audience used Q&A period to enhance their personal opinions rather than to comment or obtain an answer.
- none
- Great process will recommend to people.
- Meeting is too early for people not staying in the hotel. 9:00am - 4:00pm is more adequate.

- The ability to access the presenter's slides on the CD before the presentation and afterward when the reviews are being written is a real positive. It saves time in identifying key issues for discussions.
- It will be useful to attendees if presenters provide a 2 page extended abstract of their work/results beforehand with registration materials.
- Good technical review cannot occur in most of the areas covered in 30 minutes. But, it is very important and worthwhile to bring the researchers together. To foster greater information sharing, I would like to see a slide on lessons learned (some had this) and one on critical gaps - that is, "over the past year our research has shown that . . . . . is critical for the development of the hydrogen economy.
- Presentations need a set format. Otherwise everything was fine.

B. QUESTIONS 22 THROUGH 32 FOR PEER REVIEWERS ONLY

22. Information about the program/project(s) under review was provided sufficiently prior to the review session. *disagree* *agree* *1 2 3 4 5* **3.6**

23. Review instructions were provided in a timely manner. *disagree* *agree* *1 2 3 4 5* **4.0**

24. The information provided in the presentations was adequate for a meaningful review of the projects. *Disagree* *agree* *1 2 3 4 5* **3.4**

25. The evaluation criteria upon which the review was organized were clearly defined and used appropriately. *disagree* *agree*

1. Relevance	*1*	*2*	*3*	*4*	*5*	**4.2**
2. Approach	*1*	*2*	*3*	*4*	*5*	**4.2**
3. Technical Accomplishments and Progress	*1*	*2*	*3*	*4*	*5*	**4.2**
4. Technology Transfer/Collaboration	*1*	*2*	*3*	*4*	*5*	**3.5**
5. Proposed Future Research	*1*	*2*	*3*	*4*	*5*	**3.5**

26. Explanation of the questions within the criteria was clear and sufficient. *disagree* *agree*

1. Relevance	*1*	*2*	*3*	*4*	*5*	**4.0**
2. Approach	*1*	*2*	*3*	*4*	*5*	**4.2**
3. Technical Accomplishments and Progress	*1*	*2*	*3*	*4*	*5*	**4.2**
4. Technology Transfer/Collaboration	*1*	*2*	*3*	*4*	*5*	**3.8**
5. Proposed Future Research	*1*	*2*	*3*	*4*	*5*	**4.0**

27. The right criteria and weightings were used to evaluate the project(s)/program. *disagree* *agree*

1. Relevance	*1*	*2*	*3*	*4*	*5*	**3.9**
2. Approach	*1*	*2*	*3*	*4*	*5*	**4.3**
3. Technical Accomplishments and Progress	*1*	*2*	*3*	*4*	*5*	**4.1**
4. Technology Transfer/Collaboration	*1*	*2*	*3*	*4*	*5*	**4.2**
5. Proposed Future Research	*1*	*2*	*3*	*4*	*5*	**3.9**

28. During the review, reviewers had adequate access to the Principal Investigators. *disagree* *agree* *1 2 3 4 5* **3.9**

29. Information on the location and timing of the projects was adequate and easy to find. *disagree* *agree* *1 2 3 4 5* **4.4**

30. The number of projects I was expected to review was *disagree* *agree*
    a. Too many *1 2 3 4 5* **2**
    b. Too few *1 2 3 4 5* **2**
    c. About right *1 2 3 4 5* **4**

31. The reviewers in your session had the proper mix and depth of credentials for the purpose of the review. *Disagree* *agree* *1 2 3 4 5* **3.8**
    7 *Don't know their credentials*

32. Altogether, the preparatory materials, presentations, and the Question & Answer period provided sufficient depth for a meaningful review. *disagree* *agree* *1 2 3 4 5* **3.7**

C. QUESTIONS 33 THROUGH 43 FOR PRESENTERS ONLY

33. The request to provide a presentation for the review was provided sufficiently prior to the deadline for submission. *disagree* *agree* *1 2 3 4 5* **4.7**

34. Instructions for preparing the presentation were sufficient. *disagree* *agree* *1 2 3 4 5* **4.8**

35. The template for the presentation was helpful. *disagree* *agree* *1 2 3 4 5* **4.8**

36. The PDF format provided adequate functionality for my presentation. *disagree* *agree* *1 2 3 4 5* **4.8**

37. The time limit for my presentation was adequate to present the information needed by reviewers. *disagree* *agree* *1 2 3 4 5* **4.9**

38. The audio and visual equipment worked properly and were adequate. *disagree* *agree* *1 2 3 4 5* **4.8**

39.	The evaluation criteria upon which the review was organized were clearly defined and used appropriately	*disagree*				*agree*	
	1. Relevance	*1*	*2*	*3*	*4*	*5*	**4.5**
	2. Approach	*1*	*2*	*3*	*4*	*5*	**4.5**
	3. Technical Accomplishments and Progress	*1*	*2*	*3*	*4*	*5*	**4.6**
	4. Technology Transfer/Collaboration	*1*	*2*	*3*	*4*	*5*	**4.5**
	5. Proposed Future Research	*1*	*2*	*3*	*4*	*5*	**4.6**
40.	Explanation of the questions within the criteria was clear and sufficient.	*disagree*				*agree*	
	1. Relevance	*1*	*2*	*3*	*4*	*5*	**4.5**
	2. Approach	*1*	*2*	*3*	*4*	*5*	**4.5**
	3. Technical Accomplishments and Progress	*1*	*2*	*3*	*4*	*5*	**4.7**
	4. Technology Transfer/Collaboration	*1*	*2*	*3*	*4*	*5*	**4.5**
	5. Proposed Future Research	*1*	*2*	*3*	*4*	*5*	**4.6**
41.	The right criteria and weightings were used to evaluate the project(s)/program.	*disagree*				*agree*	
	1. Relevance	*1*	*2*	*3*	*4*	*5*	**4.6**
	2. Approach	*1*	*2*	*3*	*4*	*5*	**4.6**
	3. Technical Accomplishments and Progress	*1*	*2*	*3*	*4*	*5*	**4.6**
	4. Technology Transfer/Collaboration	*1*	*2*	*3*	*4*	*5*	**4.7**
	5. Proposed Future Research	*1*	*2*	*3*	*4*	*5*	**4.5**
42.	During the review, reviewers had adequate access to the Principal Investigators.	*Disagree*				*agree*	
		1	*2*	*3*	*4*	*5*	
				4.2			
43.	Altogether, the preparatory materials, presentations, and the Question & Answer period provided sufficient depth of review	*disagree*				*agree*	
		1	*2*	*3*	*4*	*5*	
				4.4			

APPENDIX D: FY 2007 MERIT REVIEW AND PEER EVALUATION MEETING: EVALUATION FORMS

DOE Hydrogen Program 2007 Annual Merit Review
Project Evaluation Form

Project Number: ______ **Reviewer:** ______

Presenter Name: ______ **Presenter Org:** ______

Provide specific, concise comments to support your evaluation -- and, write clearly please.

1. Relevance to overall DOE objectives – the degree to which the project supports the President's Hydrogen Fuel Initiative and the goals and objectives of the applicable Multi-Year RD&D plan. **(Weight = 20%)**

4 - Outstanding. Project is critical to Hydrogen Initiative and fully supports DOE RD&D objectives.
3 - Good. Most project aspects align with the Hydrogen vision and DOE RD&D objectives.
2 - Fair. Project partially supports the Hydrogen vision and DOE RD&D objectives.
1 - Poor. Project provides little support to the Hydrogen vision and the DOE RD&D objectives.

score

comments

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2. Approach to performing the R&D – the degree to which technical barriers are addressed, the project is well-designed, technically feasible, and integrated with other research. **(Weight = 20%)**

4 - Outstanding. Sharply focused on technical barriers; difficult to improve approach significantly.
3 - Good. Generally effective but could be improved; contributes to overcoming some barriers.
2 - Fair. Has significant weaknesses; may have some impact on overcoming barriers.
1 - Poor. Not responsive to project objectives; unlikely to contribute to overcoming the barriers.

score

comments

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3. Technical Accomplishments and Progress toward overall project and DOE goals – the degree to which research progress is measured against performance indicators and to which the project elicits improved performance (effectiveness, efficiency, cost, and benefits). **(Weight = 35%)**

4 - Outstanding. Excellent progress toward objectives; suggests that barrier(s) will be overcome.
3 - Good. Significant progress toward objectives and overcoming one or more barriers.
2 - Fair. Modest progress in overcoming barriers; rate of progress has been slow.
1 - Poor. Little or no demonstrated progress towards objectives or any barriers.

score

comments

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Page 1 of 2

4. Technology Transfer/Collaborations with industry/universities/other laboratories – the degree to which the project interacts, interfaces, or coordinates with other institutions and projects. **(Weight = 10%)**

4 - Outstanding. Close, appropriate coordination with other institutions; partners are full participants.
3 - Good. Some coordination exists; full/needed coordination could be accomplished easily.
2 - Fair. A little coordination exists; full/needed coordination would take significant effort.
1 - Poor. Most work is done at the sponsoring organization with little outside interaction.

score

comments

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5. Proposed Future Research approach and relevance – the degree to which the project has effectively planned its future, considered contingencies, built in optional paths or off ramps, etc. **(Weight = 15%)**

4 - Outstanding. Plans clearly build on past progress and are sharply focused on barriers.
3 - Good. Plans build on past progress and generally address overcoming barriers.
2 - Fair. Plans may lead to improvements, but need better focus on overcoming barriers.
1 - Poor. Plans have little relevance toward eliminating barriers or advancing the program.

score

comments

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Project Strengths

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Project Weaknesses

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Recommendations for Additions/Deletions to Project Scope

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Project Number: | **Reviewer:**

Page 2 of 2

DOE Hydrogen Program
2007 Annual Merit Review

Sub-Program Evaluation Form

Reviewer:

Title of Sub-Prog:

Presenter Name:

Using the following criteria, rate the work presented in the context of the program objectives and provide **specific, concise** comments to support your evaluation. *** Write/print **clearly** please. ***

1. Degree to which the Sub-Program area was adequately covered and/or summarized:

2. Were important problem/issue areas and challenges identified/discussed, including plans for addressing these in the future?:

3. Does the Sub-Program area appear to be focused, managed well, and effective in addressing the DOE Hydrogen Program R&D needs?:

4. Other Comments:

Page 1 of 1

DOE Hydrogen Program
2007 Annual Merit Review and Peer Evaluation Meeting
Hydrogen Storage Center of Excellence Evaluation Form

NOTE: This evaluation form is only for the evaluation of the Center of Excellence overall presentation (NOT for partner evaluations)

Project Number:		Reviewer Name:	
Title of Project:		Center of Excellence Overall Presentation	

(Sorption, Metal Hydride, or Chemical)

Using the following criteria, rate the work presented in the context of the program objectives and provide specific, concise comments to support your evaluation.

1. Approach to performing the R&D – the degree to which the DOE EERE Multi-year Program Plan (RD&D Plan) technical barriers are addressed; the overall CoE effort is well-designed and technically feasible. The technical approach clearly leverages partners' unique skills to complement activities and avoid duplication. The CoE management approach includes, and has demonstrated, effective down-select/decision points and criteria. CoE progress and technical direction are periodically internally "audited" for effectiveness, efficiency, and benefits.
(Weight = 25%)

4 - Outstanding. The overall center is sharply focused on one or more key technical barriers to development of onboard hydrogen storage technology (focused on 2010 targets). Difficult for the approach to be improved significantly.

3 - Good. The approach is generally well thought out and effective but could be improved in a few areas. Most aspects of the center projects will contribute to progress in overcoming the barriers.

2 - Fair. Some aspects of the center projects may lead to progress in overcoming some barriers, but the approach has significant weaknesses.

1 - Poor. The approach is not responsive to project objectives and unlikely to make significant contributions to overcoming the barriers.

score	**comments**

2. Technical accomplishments and progress toward DOE goals – the degree to which the CoE research has achieved progress across the center. CoE's actual progress and technical accomplishments are measured against performance indicators and quantitative milestones as related to DOE's RD&D plan.
(Weight = 25%)

4 - Outstanding. The overall CoE has made excellent progress toward objectives and overcoming one or more key technical barriers. Progress to date suggests that the barrier(s) may be overcome.

3 - Good. The overall CoE has shown significant progress toward its objectives and to overcoming one or more technical barriers.

2 - Fair. The overall CoE has shown modest progress in overcoming barriers, and the rate of progress has been slow.

1 - Poor. The overall CoE has demonstrated little or no progress towards its objectives or any barriers.

score comments

3. Proposed future research approach and relevance – the degree to which the CoE has effectively planned its future, considered contingencies, built in optional paths or off ramps, etc. (Weight = 20%)

4 - Outstanding. The future work plan clearly builds on past progress and is sharply focused on one or more key technical barriers in a timely manner.

3 - Good. Future work plans build on past progress and generally address removing or diminishing barriers in a reasonable period.

2 - Fair. The future work plan may lead to improvements, but should be better focused on removing/diminishing key barriers in a reasonable timeframe.

1 - Poor. Future work plans have little relevance or benefit toward eliminating barriers or advancing the program.

score comments

4. Coordination, collaborations and effectiveness of communications within the CoE – the degree to which the partners interact, interface, or coordinate with other partners within the CoE. The center coordinator provides a mechanism to foster partner interaction, interface, or coordination within the CoE. The center coordinator has helped to leverage resources to achieve progress and obtained maximum benefit from the center's overall funding. Technical progress gained from the CoE has benefited from the group effort as opposed to a group of independent projects.
(Weight = 20%)

4 - Outstanding. Close coordination is evident among the majority of partners with continuing cross center communications and collaborations; partners are full participants.

3 - Good. Some coordination exists; full and needed coordination could be accomplished fairly easily.

2 - Fair. A little coordination exists; full and needed coordination would take significant time and effort to initiate. Some partners appear to be insufficiently aware of other work occurring in the CoE.

1 - Poor. Communications among and between partners appears to be insufficient. It appears as if unnecessary duplication of work may be occurring.

score	comments

5. Collaborations/Technology Transfer Outside the CoE – the degree to which the CoE interacts, interfaces, or coordinates with the other DOE CoEs and with other institutions and projects.
(Weight = 10%)
4 - Outstanding. Close coordination with other DOE CoEs and other institutions is in place and appropriate; the CoE is formally leveraging other work occurring in the subject areas.
3 - Good. Some coordination exists; full and needed coordination could be accomplished fairly easily.
2 - Fair. A little coordination exists; full and needed coordination would take significant time and effort to initiate. The CoE does not appear to be fully aware of other major R&D efforts occurring in a particular subject area.
1 - Poor. Most of the work done within the CoE; has little outside interactions or collaborations.

score	comments

Overall Center Strengths

Overall Center Weaknesses

Recommendations for Additions/Deletions to Center Scope

Project # AN: Systems Analysis
Fred Joseck; Systems Analysis

Degree to which the Sub-Program area was adequately covered and/or summarized

- Model and analysis matrix shown does an excellent job of putting this subprogram in perspective. Matrix of the models and their function was especially useful.

Were important problem/issue areas and challenges identified/discussed, including plans for addressing these items in the future?

- Although this subprogram lists barriers that must be addressed, its most important contribution is the evaluation of technical and market barriers for the balance of the Program and prioritization of those barriers. Future market behavior is a barrier that is included in the MYPP, but the systems analysis subprogram should take credit for its efforts to understand the technical barriers and their relative priority within the Program.

Does the Sub-Program area appear to be focused, managed well, and effective in addressing the Hydrogen Program R&D needs?

- Models are well focused on understanding the barriers, in particular the market barriers that must be addressed. Use of the models will enable DOE to prioritize those barriers and evaluate where they RD&D funding can be used to reduce those barriers.

Other comments:

- The MYPP for Systems Analysis lists "Inconsistent data, assumptions and guidelines" as a barrier. One area to consider for future work is to focus on resolving these inconsistencies and/or understanding the variations.
- It may be too soon to attempt to add the cost of safety to the models, but it is not too early to evaluate the impact of consumer perception of safety and its impact on market penetration.
- Many of the models have not been validated. Consideration should be given to include a requirement for each project to develop a validation plan during the next FY.

Project # ED: Education
Christy Cooper; Education

Degree to which the Sub-Program area was adequately covered and/or summarized

- Very well

Were important problem/issue areas and challenges identified/discussed, including plans for addressing these items in the future?

- Yes — plans for increasing target audience knowledge of hydrogen.

Does the Sub-Program area appear to be focused, managed well, and effective in addressing the Hydrogen Program R&D needs?

- Yes — accomplished a lot with zero or limited funds.

Other comments:

Project # FC: Fuel Cells
Nancy Garland; Fuel Cells

Degree to which the Sub-Program area was adequately covered and/or summarized

- Excellent overview.
- Pretty quick, due to the short time allotted and the late start, but still was adequate.

Were important problem/issue areas and challenges identified/discussed, including plans for addressing these items in the future?

- Yes.
- Yes, cost and durability are definitely the primary barriers.
- Nice to water transport/management within the stack is finally getting the attention it deserves. This must be understood and effectively dealt with in order to meet the cost and durability targets.

Does the Sub-Program area appear to be focused, managed well, and effective in addressing the Hydrogen Program R&D needs?

- Yes, there is a nice portfolio of membrane projects, although this is a difficult area and you probably can never have enough. More funding should be requested for Non-Pt or ultra low Pt and non-carbon electrodes. This issue is as important as the membrane issue and no one should be kidding themselves that Pt costs will stay low or will be achieved under real manufacturing conditions.
- Yes. The EERE team has consistently listened to fuel-cell developers, component suppliers, and other involved parties, regarding what the challenges are going forward and have adjusted the fuel-cell program accordingly. This review meeting is one good example of that continuous improvement process.

Other comments:

- How will 40,000 h for Distributed Energy be demonstrated by 2011? Since that is 5 years of run time, the demonstration should already be underway. Is it underway, or is the goal that a projection to 40k h, with some high degree of confidence (e.g., based on accelerated testing), can be made by that date?
- One project that does not appear to fit DOE's goals and their stated position on PAFC (no funding) is FC-8. PBI doped with phosphoric acid is essentially a PAFC -- look at the polarization curve and the issues associated with losing electrolyte, they both stink and make meeting the cost and lifetime goals very challenging. DOE's position to not fund PAFC is a good one, since the money is better spent looking for a better high temperature electrolyte, preferably a true polymer electrolyte or a solid electrolyte. If an electrolyte has a vapor pressure, it is not a polymer. Beware of a wolf in sheep's clothing.

Project # ST: Hydrogen Storage
Sunita Satyapal; Hydrogen Storage

Degree to which the Sub-Program area was adequately covered and/or summarized

- Excellent overview of the sub-program area, of its strategy, technical goals and main achievements.
- A nice description of the program and its goals and rationale for approach. Obviously with 70 some projects they could not all be touched on specifically. Good description of progress to date and plans for the future.
- The overview was good and largely complete in discussing the needs (targets), activities, progress and future plans.
- The overview was complete and accurate with chief achievement descriptions. The presentation gave clear insight of the progress, the expectations and plans.
- The coverage of the issues by the presenter was thorough and clear.
- The sub-program was organized and well-covered, a large achievement given the amount of information, projects, and diversity of topics. The format of the talk addressed the key aspects, enabling reviewers/participants to understand the objectives, technical progress, program structure, and future work. Both short- and long-term goals/plans were also shown and are indicative of a balanced perspective on both details and broad scope.
- Good coverage of the storage program.
- More emphasis needed on system requirements and especially infrastructure issues particularly when it comes to cryogenic temperature.

Were important problem/issue areas and challenges identified/discussed, including plans for addressing these items in the future?

- Both issues and plans were made clear. A nice set up for the individual project talks to come which will no doubt reference these same issues - but in telegraphic form - allowing them more time to discuss what we need to hear, approach, progress and plans. The plans for the engineering center are less than fully defined at this point, but at lest the general rational and direction were clear enough.
- There was a good discussion of capacity, kinetics, and delta H and release temperature as key challenges.
- Critical areas and challenges were discussed along with short and longer term plans for attacking them. Important milestones and decision points were presented and so were the results of recent solicitations and the announcement for an expression of interest for a new CoE on engineering issues
- Problems and issues were discussed in some detail: theory assisted materials development, system properties (weight, volume, recharging times, cost, etc.), safety, testing of prototypes, etc. Future efforts and funding requests outlined for long-term efforts to assault the technical barriers. The three CoEs were discussed in terms of their valuable coordination of collaborative activities. An engineering CoE is a good idea.
- The major technical issues have been identified and presented for an open discussion and updating. Of special interest is the focus of the operation and effectiveness of the CoE under revision and the intention to give more emphasis to engineering aspects.
- The considerable challenges facing the storage R&D activities were clearly expressed by the gravimetric vs. volumetric summary figures. Perhaps I could suggest mentioning in the project summary part to state at some point on a slide that the storage densities presented are material capacities. The future plans were clearly summarized at the end of the presentation.
- It was especially useful for common issues to be clarified, for example, reiterating that the storage targets are 'system' and not 'materials' based. Acknowledgement of the difficulty and challenges that are inherent to this research area also helped to motivate and incite optimism. Additionally, clear (go/no-go) decision points were also presented to ensure a roadmap focused on progress is in place.
- Given the limited time, yes in general all important issues were highlighted.
- It is recommended to start emphasizing safety, and toxicity issues for the benefits of all researchers and how it will be used in down-selecting process.
- More emphasis needed on how various storage alternatives affect the infrastructure (well-to-wheel) energy efficiency.

Does the Sub-Program area appear to be focused, managed well, and effective in addressing the Hydrogen Program R&D needs?

- The Storage sub-program is very well focused, with a robust R&D portfolio and clear ties to technical targets and overall efficiently managed.
- The program is extremely well managed and effective in meeting very difficult technology challenges. In particular, the center of excellence approach on each main topic is an excellent and efficient way to pool resources for the R&D and provide clear focus to the participants. Of particular interest is the new Engineering Center of Excellence, which will help address systems issues often neglected by the other centers, and provide some insight on the overall efficiency, cost and thermal management strategies of the storage systems using the various unconventional storage strategies.
- Yes. This sub-program is extremely well-managed. There is a sharp focus on the targets, maintained communication between the program management/tech-team and the projects/CoEs, and a willingness/ eagerness to adapt to an evolving and progressing field.
- I feel the DOE team managing hydrogen storage is excellent, and that it is well managed at all levels, not just the level of the presenter. The large and complex task of monitoring the 70 to 80 actual projects (which are required to achieve success with any likelihood) have been grouped into several centers which manage them on a day to day, month to month basis. This allows the management team to focus on a more tractable number of large programs on a day to day and month to month basis, while still retaining the right to investigate progress on individual projects on a more infrequent basis and as needed.
- The selection of programs has been managed well. While a few doubtful projects have been started based on independent reviewers who may not have been well suited to their task, the management team has swiftly isolated those few less appropriate programs and de-funded them so the money available can be focused on productive programs.
- Also despite pressure to focus on many different researchers' pet programs, the management team has held firm to a wide scope until there is significant evidence of a path to solution. They are also self critical and evaluate for example how the centers feel the DOE management is doing.
- Probably the best managed of the subprograms.
- The program is well focused and managed. There are good interactions with BES, FreedomCAR, IPHE, IEA, etc. Progress is nicely mapped and reasonable go/no-go decision points in place.
- The Subprogram remains central in the DOE Program.
- The focus is on key scientific aspects with increased attention, in terms of subprogram efforts (not only targets), to a system approach.
- The management is well motivated and organized with new support from well known and experienced consultants able to enlarge the analysis capacity to better address R&D needs.
- The managing of the program is good.
- Need to develop more flexible strategies to accommodate new data.
- If not already, need to start a review of the portfolio and assess the progress to date.
- The transition scenario analysis showed the effect of storage cost targets on the FCV (fuel cell vehicle) penetration. How much of this information is shared with the researchers?

Other comments:

- H_2 storage has been a driver in inter-team communication, and was so before it was a focus handed to FreedomCAR by the peer review. They have also been highly engaged in coordination with international groups. There are few if any opportunities to improve and leverage their program that they are not currently using.
- The team is responsive and approachable. They have a huge task and are making progress despite the fact I feel they are well understaffed for the job at hand. It is quite beneficial that the manager (Satyapal) is directly involved in all phases, the management of the budget and oversight team, the leadership of the 'technical reference team,' the people in FreedomCAR who critique all the programs, and direct reporting to the DOE management. By doing all these jobs there is automatic coordination which is absolutely crucial to completing this mission. She needs to have sufficient support so she can maintain these many tasks and her sanity. Any other approach will be less effective.
- Maintain independent projects to ensure flexibility and agility.

- Ensure transparency on the methods of CoE operation and management (structure, decision process, meetings, communication flow & synergy among the sub-program areas, IPR management).
- Establish interaction mechanisms among the CoEs for sharing experiences and lessons learned particularly on cross-cutting issues - not yet clear how this currently works.
- Engineering issues and tank system design could be further emphasized and the PIs should be encouraged to address them earlier on in the program.
- Keep reminding PIs that they need to address system rather than material targets and also engineering aspects and not just gravimetric capacities.
- Almost all projects have been made to conform to DOE multi-year RD&D plan targets for 2010 and/or 2015.
- It would be interesting to look at different strategies beyond storage density optimization in order to achieve the autonomy expected of hydrogen vehicles. Should we factor in vehicle weight objectives, for instance? I hope such issues will be addressed by the new engineering center, through, for instance, a system analysis that could identify what weight reduction strategy in vehicle infrastructure would be required to achieve consumer acceptable driving range for hydrogen powered vehicles.
- If not already, it is recommended to start a formal review of the portfolio and assess the progress to date.
- What was learned by the outcome maps or (gap analysis)? How does that match with the actual progress metrics to date?
- The transition scenario analysis showed the effect of storage cost targets on the FCV penetration. How much of this information is shared with the researchers? And in general, how much of the project researchers are aware of the cross-cutting impacts of storage on the entire hydrogen chain?

Project # TV: Technology Validation
John Garbak; Technology Validation

Degree to which the Sub-Program area was adequately covered and/or summarized

- Mr. Garbak provided an excellent summary of a sub-program having a number of important elements.
- Easy-to-grasp budget overview for FY 2007/2008. Clearly identified major areas receiving funds.
- Could have provided more summary data, e.g., total miles.

Were important problem/issue areas and challenges identified/discussed, including plans for addressing these items in the future?

- The major challenges were summarized.
- There was limited discussion of plans for dealing with the challenges. Could have included a few specific examples of both challenges and plans.
- Overall "Good".

Does the Sub-Program area appear to be focused, managed well, and effective in addressing the Hydrogen Program R&D needs?

- Bulk of the DOE funds are used to address transportation issues. The Hydrogen Program Manager should consider increasing the resources devoted to projects that demonstrate and validate integrated systems for stationary applications of hydrogen. Many of those are expected to be economic and commercially competitive before transportation.

Other comments:

- Mr. Garbak's overview provided an excellent lead-in to the more detailed presentations that followed his.